NCASO Spring 2015

Complexity à la Mode: Spectral Methods for Complex Systems Part $e^{i\omega}\big|_{\omega=0}$

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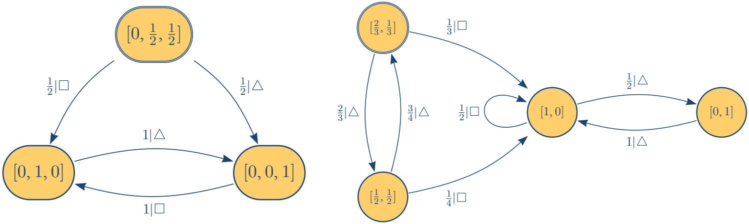
Visualizing Modes



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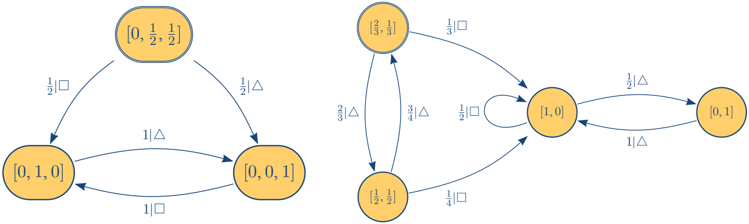

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Spectral methods formalize and empower our intuition.

Sample of Exact Results Obtained in Closed-Form:

Directly from *any* HMM presentation of a process:

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Directly from MSP of ϵ-machine:

- Average causal-state uncertainty $\mathcal{H}(L)$
- Synchronization Information $\mathbf{S}$

HMMs as Mathematical Objects

(Autonomous) Process specified by $\mathcal{A}$, $T^{\mathcal{A}}$, and μ_0

- $T^{\mathcal{A}^*}$ together with the identity I form a semigroup
- The spectral properties of T, $T^{\mathcal{A}}$, and functions of $T^{\mathcal{A}}$ (e.g., MSP) describe the modes of probability density and information flows

Any HMM will have:

- some set of states $\boldsymbol{\mathcal{S}}$,
- an alphabet $\mathcal{A}$ of observables,
- a set of $|\boldsymbol{\mathcal{S}}|$-by-$|\boldsymbol{\mathcal{S}}|$ labeled transition matrices $T^{\mathcal{A}} = \{T^{(x)} : T^{(x)}_{i,j} = \Pr(\mathcal{S}_t = \sigma^j | \mathcal{S}_{t-1} = \sigma^i)\}_{x \in \mathcal{A}}$ constituting the row-stochastic state-to-state transition matrix $T = \sum_{x \in \mathcal{A}} T^{(x)}$.

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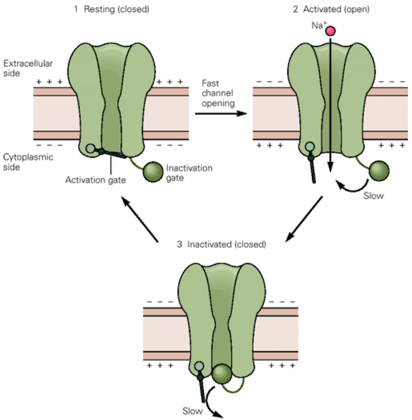
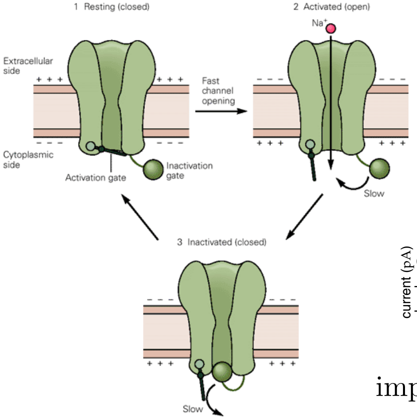
Note:

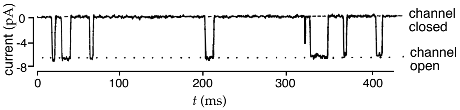
- bra–ket notation:
  - $|\mathbf{1}\rangle$ is the column vector of all ones
  - π is the stationary distribution over $\boldsymbol{\mathcal{S}}$; when cast as a row-vector: $\langle \pi | = \langle \pi | T$
- length-n 'word' $w = x_0 x_1 \ldots x_{n-1} \in \mathcal{A}^n$
- Probability of observing w given initial distribution μ over $\boldsymbol{\mathcal{S}}$ is: $\Pr_\mu(w) \equiv \Pr(X_{0:n} = w | S_0 \sim \mu) = \langle \mu | T^{(w)} | \mathbf{1} \rangle = \langle \mu | T^{(x_0)} T^{(x_1)} \ldots T^{(x_{n-1})} | \mathbf{1} \rangle$.
- Stationary probability of w is: $\Pr(w) = \langle \pi | T^{(w)} | \mathbf{1} \rangle$.
- $X_{0:n}$ is left-inclusive and right-exclusive.



'hidden' conformational states $\sim \boldsymbol{\mathcal{S}}$

figures from Koester&Siegelbaum and Dayan&Abbott





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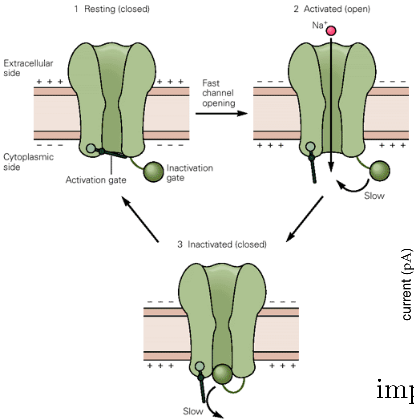

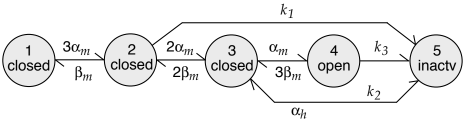

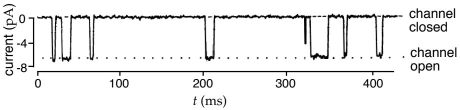

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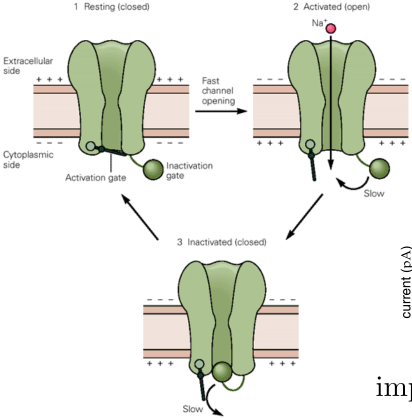

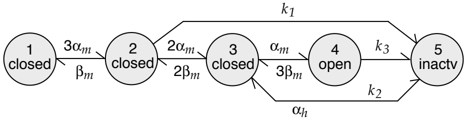

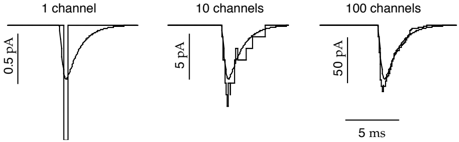

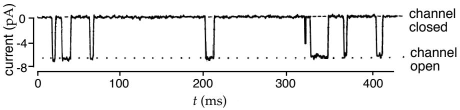

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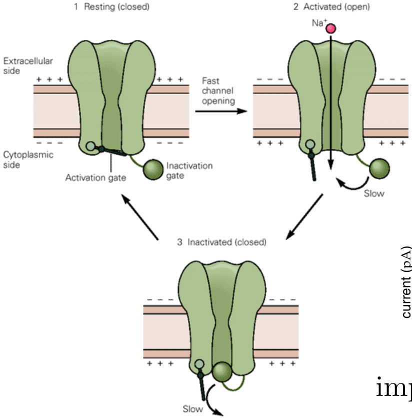
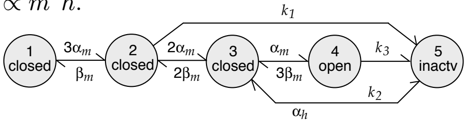
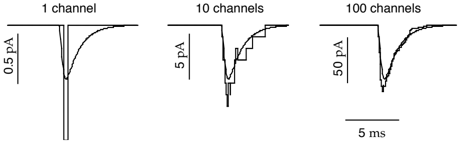
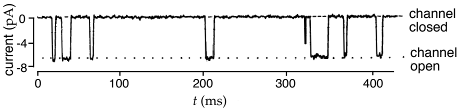
Recall that H–H model is acausal: $I^{\text{H–H}}_{\text{Na}^+} \propto m^3 h$.
Consequences?!









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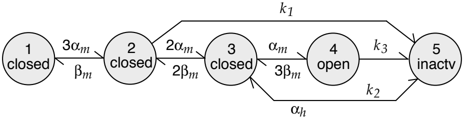
Notation and Methods via Ion Channel Dynamics



$$\mathcal{A} = \{0 = \text{`OFF'}, 1 = \text{`ON'}\}$$

$$T^{(0)}(v, \Delta t) = \begin{bmatrix} 1 - 3\alpha_m \Delta t & 3\alpha_m \Delta t & 0 & 0 & 0 \\ \beta_m \Delta t & 1 - (2\alpha_m + \beta_m + k_1)\Delta t & 2\alpha_m \Delta t & 0 & k_1 \Delta t \\ 0 & 2\beta_m \Delta t & 1 - (\alpha_m + 2\beta_m + k_2)\Delta t & 0 & k_2 \Delta t \\ 0 & 0 & 3\beta_m \Delta t & 0 & k_3 \Delta t \\ 0 & 0 & \alpha_h \Delta t & 0 & 1 - \alpha_h \Delta t \end{bmatrix}$$

$$T^{(1)}(v, \Delta t) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \alpha_m \Delta t & 0 \\ 0 & 0 & 0 & 1 - (3\beta_m + k_3)\Delta t & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

where the α_m, β_m, and α_h are the voltage-dependent variables as in the Hodgkin and Huxley model.

Causally structured model of voltage-gated Na^+ channel

The state-to-state transition matrix is:

$$T(v, \Delta t) = T^{(0)}(v, \Delta t) + T^{(1)}(v, \Delta t)$$

$$= I + (\Delta t) G(v) \quad ,$$

where I is the identity matrix and

$$G(v) \equiv \begin{bmatrix} -3\alpha_m & 3\alpha_m & 0 & 0 & 0 \\ \beta_m & -(2\alpha_m + \beta_m + k_1) & 2\alpha_m & 0 & k_1 \\ 0 & 2\beta_m & -(\alpha_m + 2\beta_m + k_2) & \alpha_m & k_2 \\ 0 & 0 & 3\beta_m & -(3\beta_m + k_3) & k_3 \\ 0 & 0 & \alpha_h & 0 & -\alpha_h \end{bmatrix} .$$

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In applying a voltage step from -100mV to 10mV, the average current flowing through a channel is:

$$\langle I(t = n\Delta t)\rangle$$
$$= \sum_{w \in \mathcal{A}^{n-1}} \left[I_0 \Pr_\mu(w) \Pr_\mu(X_n = 1 | X_{0:n} = w) + 0 \Pr_\mu(w) \Pr_\mu(X_n = 0 | X_{0:n} = w) \right]$$

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\end{aligned}
$$

Causally structured model of voltage-gated Na^+ channel

So,

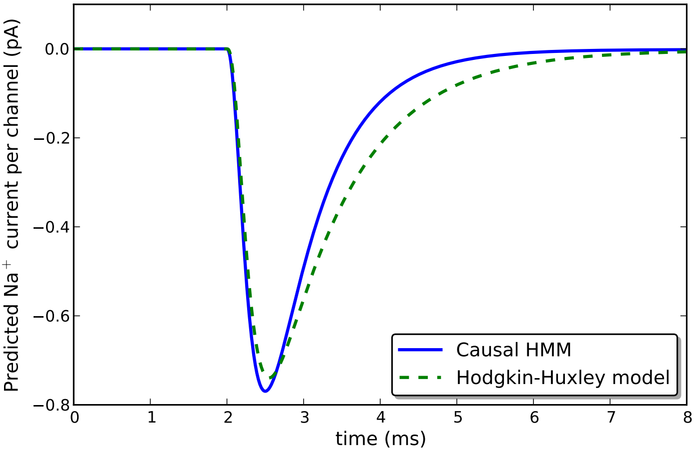
$$\langle I(t = n\Delta t)\rangle \quad = I_0 \langle \mu| T^{n-1} T^{(1)} |\mathbf{1}\rangle ,$$

and

$$\begin{aligned} \lim_{\substack{\Delta t \to 0 \\ n\Delta t = t}} T^n(v = V, \Delta t) &= \lim_{\substack{\Delta t \to 0 \\ n\Delta t = t}} [I + (\Delta t)G]^n \\ &= \lim_{\Delta t \to 0} [I + (\Delta t)G]^{t/(\Delta t)} \\ &= e^{G\,t}, \end{aligned}$$

yielding $\langle I(t)\rangle = I_0 \langle \pi_{-100\text{ mV}}| e^{t\,G(v=V)} |(0,0,0,1,0)\rangle$ as the continuous-time result.

Causally structured model of voltage-gated Na^+ channel



An Operator and its Spectrum

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Resolvent

The *resolvent* of A, $\mathcal{R}(z; A) \equiv (zI - A)^{-1}$, where z is a continuous complex variable, thus contains all of the spectral information about A (and more).

A finite square matrix and its eigenvalues

- If an operator A can be represented as a finite square matrix, then its spectrum is just the set of A's *eigenvalues*:

$$\Lambda_A \equiv \{\lambda \in \mathbb{C} : \det(\lambda I - A) = 0\}$$

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- Compare the algebraic multiplicity a_λ, geometric multiplicity g_λ, and index ν_λ of the eigenvalue λ:

$$\nu_\lambda - 1 \leq a_\lambda - g_\lambda \leq a_\lambda - 1 \ .$$

Definition

Projection Operator

The *projection operator* of A associated with the eigenvalue λ is:

$$A_\lambda \equiv \frac{1}{2\pi i} \oint_{C_\lambda} \mathcal{R}(z; A)\, dz$$
$$= \text{Res}\left[(zI - A)^{-1}, z \to \lambda\right]$$

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If $a_\lambda = 1$, then the projection operator can be simply expressed as:

$$A_\lambda = \frac{1}{\langle \boldsymbol{\lambda} | \boldsymbol{\lambda} \rangle} |\boldsymbol{\lambda}\rangle \langle \boldsymbol{\lambda}| \ ,$$

where $\langle \boldsymbol{\lambda}|$ is the left eigenvector of A associated with λ and $|\boldsymbol{\lambda}\rangle$ is the right eigenvector of A associated with λ. (Note: $\langle \boldsymbol{\lambda}| \neq |\boldsymbol{\lambda}\rangle^\dagger$!)

Some General Properties of Projection Operators

- $\{A_\lambda\}$ is a mutually orthogonal set:

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- The projection operators are a resolution of the identity:

$$I = \sum_{\lambda \in \Lambda_A} A_\lambda$$

The Resolvent Resolved

Partial Fraction Decomposition of the Resolvent:

$$\begin{aligned}
\mathcal{R}(z;A) &= (zI-A)^{-1} \\
&= \frac{\mathcal{C}^\top}{\det(zI-A)} \\
&= \frac{\mathcal{C}^\top}{\prod_{\lambda\in\Lambda_A}(z-\lambda)^{a_\lambda}} \\
&= \sum_{\lambda\in\Lambda_A}\sum_{m=0}^{a_\lambda-1}\frac{1}{(z-\lambda)^{m+1}}A_{\lambda,m} \\
&= \sum_{\lambda\in\Lambda_A}\sum_{m=0}^{\nu_\lambda-1}\frac{1}{(z-\lambda)^{m+1}}A_\lambda\big(A-\lambda I\big)^m
\end{aligned}$$

for $z \notin \Lambda_A$, where $\mathcal{C}$ is the matrix of cofactors of $zI - A$.

Functions of Square Matrices

Cauchy integral formula

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Functions of Diagonalizable Matrices

If A is diagonalizable and $f(z)$ has no poles or zeros at Λ_A, then

$$f(A) = \sum_{\lambda \in \Lambda_A} f(\lambda) A_\lambda,$$

where

$$A_\lambda = \prod_{\substack{\zeta \in \Lambda_A \\ \zeta \neq \lambda}} \frac{A - \zeta I}{\lambda - \zeta}.$$

Powers of Matrices

$$A^L = \sum_{\lambda \in \Lambda_A \setminus \{0\}} \lambda^L A_\lambda \left[I + \sum_{m=1}^{\nu_\lambda - 1} \binom{L}{m} \left(\lambda^{-1} A - I \right)^m \right]$$
$$+ [0 \in \Lambda_A] \left[\sum_{m=0}^{\nu_0 - 1} \delta_{L,m} A_0 A^m \right]$$

for any $L \in \mathbb{C}$, where $\binom{L}{m}$ is the generalized binomial coefficient:

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With the allowance that $0^n = \delta_{n,0}$, A^L can be written as:

$$A^L = \sum_{\lambda \in \Lambda_A} \sum_{m=0}^{\nu_\lambda - 1} \binom{L}{m} \lambda^{L-m} A_\lambda (A - \lambda I)^m \ .$$

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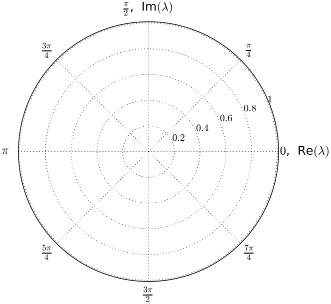

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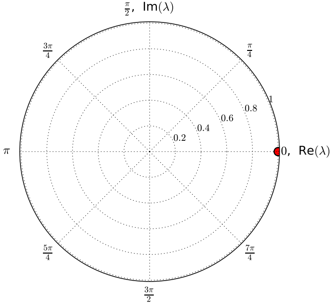

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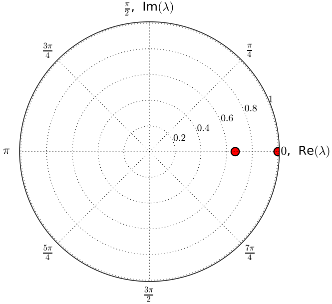

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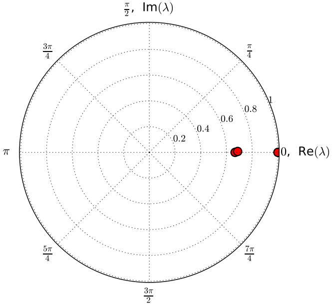

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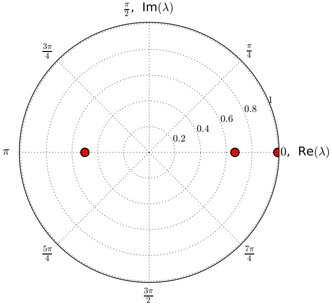

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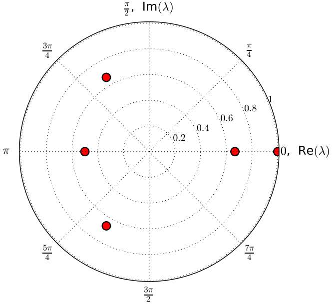
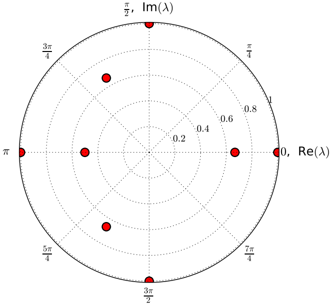


For a real-valued stochastic square matrix T:

- The largest eigenvalue(s) of T have unity magnitude
- Unity itself is guaranteed to be an eigenvalue of W with $g_1 = a_1$
- Complex eigenvalues of T must occur in complex conjugate pairs
- Eigenvalues of T that appear on the unit circle must be roots of unity and correspond to persistent periodic behavior in one of the attractors



Projection Operators for Stochastic Transition Matrices

- T_1 is row-stochastic; all other projection operators are row-zero:

$$T_\lambda \left|\mathbf{1}\right\rangle = \delta_{\lambda,1} \left|\mathbf{1}\right\rangle$$

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- For non-ergodic processes, the expected stationary distribution $\langle\pi_\alpha|$ to arise from any initial distribution α is simply

$$\langle\pi_\alpha| = \langle\alpha| \, T_1$$

Autocorrelation function

The *autocorrelation function* can be expressed as

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where, e.g.:

$$\begin{aligned}
\mathrm{E}\{\overline{X}_n X_{n+\tau}\}_{(\tau>0)} &= \sum_{s\in\mathcal{A}} \sum_{s'\in\mathcal{A}} \overline{s}s' \Pr(X_n = s, X_{n+\tau} = s') \\
&= \sum_{s\in\mathcal{A}} \sum_{s'\in\mathcal{A}} \overline{s}s' \Pr(s \underbrace{*\cdots*}_{\tau-1\ *\mathrm{s}} s') \\
&= \sum_{s\in\mathcal{A}} \sum_{s'\in\mathcal{A}} \overline{s}s' \sum_{w\in\mathcal{A}^{\tau-1}} \Pr(sws') \\
&= \sum_{s\in\mathcal{A}} \sum_{s'\in\mathcal{A}} \overline{s}s' \sum_{w\in\mathcal{A}^{\tau-1}} \langle\pi|T^{(s)}T^{(w)}T^{(s')}|1\rangle \\
&= \sum_{s\in\mathcal{A}} \sum_{s'\in\mathcal{A}} \overline{s}s' \langle\pi|T^{(s)}\Big(\sum_{w\in\mathcal{A}^{\tau-1}} T^{(w)}\Big)T^{(s')}|1\rangle \\
&= \sum_{s\in\mathcal{A}} \sum_{s'\in\mathcal{A}} \overline{s}s' \langle\pi|T^{(s)}\Big(\prod_{i=1}^{\tau-1} \underbrace{\sum_{s_i\in\mathcal{A}} T^{(s_i)}}_{=T}\Big)T^{(s')}|1\rangle \\
&= \sum_{s\in\mathcal{A}} \sum_{s'\in\mathcal{A}} \overline{s}s' \langle\pi|T^{(s)}T^{\tau-1}T^{(s')}|1\rangle \\
&= \langle\pi|\Big(\sum_{s\in\mathcal{A}} \overline{s}T^{(s)}\Big)T^{\tau-1}\Big(\sum_{s'\in\mathcal{A}} s'T^{(s')}\Big)|1\rangle,
\end{aligned}$$

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The *autocorrelation function* can be expressed as

$$\begin{aligned}
\gamma[\tau] &\equiv \left\langle \, \overline{X_n} \, X_{n+\tau} \, \right\rangle_n \\
&= \delta[\tau] \, \langle \pi | \left(\sum_{x \in \mathcal{A}} |x|^2 T^{(x)} \right) |\mathbf{1}\rangle \\
&\quad + \; u[\tau - 1] \;\; \langle \pi | \left(\sum_{x \in \mathcal{A}} \overline{x} T^{(x)} \right) T^{\tau - 1} \left(\sum_{x' \in \mathcal{A}} x' T^{(x')} \right) |\mathbf{1}\rangle \\
&\quad + u[-\tau - 1] \, \langle \pi | \left(\sum_{x \in \mathcal{A}} x T^{(x)} \right) T^{-\tau - 1} \left(\sum_{x' \in \mathcal{A}} \overline{x'} T^{(x')} \right) |\mathbf{1}\rangle \, .
\end{aligned}$$

which is an even function of τ.

Power Spectrum

The continuous part of the *power spectrum* of a process is

$$P_{\mathrm{c}}(\omega) = \lim_{N\to\infty} \frac{1}{N} \left\langle \left| \sum_{n=1}^{N} X_n e^{-i\omega n} \right|^2 \right\rangle$$

$$= \lim_{N\to\infty} \frac{1}{N} \sum_{L=-N}^{N} (N - |L|)\gamma(L) e^{-i\omega L}$$

$$= \langle\pi| \left(\sum_{x\in\mathcal{A}} |x|^2 T^{(x)} \right) |\mathbf{1}\rangle + 2\mathrm{Re}\Bigg\{ \langle\pi| \left(\sum_{x\in\mathcal{A}} \overline{x} T^{(x)} \right)$$

$$\times (e^{i\omega} I - T)^{-1} \left(\sum_{x'\in\mathcal{A}} x' T^{(x')} \right) |\mathbf{1}\rangle \Bigg\}.$$

Note that $(e^{i\omega} I - T)^{-1}$ is $\mathcal{R}(z;T)\big|_{z=e^{i\omega}}$.

Power Spectrum

If $\mathcal{A} = \{0, 1\}$, then the power spectrum is simply:

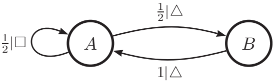
$$P_c(\omega) = \langle \pi | T^{(1)} | \mathbf{1} \rangle + 2\mathrm{Re} \langle \pi | T^{(1)} (e^{i\omega} I - T)^{-1} T^{(1)} | \mathbf{1} \rangle .$$

Moreover, if T is diagonalizable, then:

$$(e^{i\omega} I - T)^{-1} = \sum_{\lambda \in \Lambda_T} \frac{1}{e^{i\omega} - \lambda} T_\lambda ,$$

yielding:

$$P_c(\omega) = \langle \pi | T^{(1)} | \mathbf{1} \rangle + 2 \sum_{\lambda \in \Lambda_T} \mathrm{Re} \frac{\langle \pi | T^{(1)} T_\lambda T^{(1)} | \mathbf{1} \rangle}{e^{i\omega} - \lambda} .$$



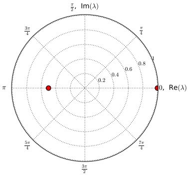
$$T^{(0)} = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & 0 \end{bmatrix} \text{ and } T^{(1)} = \begin{bmatrix} 0 & \frac{1}{2} \\ 1 & 0 \end{bmatrix} \to T = T^{(0)} + T^{(1)} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ 1 & 0 \end{bmatrix}.$$

$$\Lambda_T = \{\lambda \in \mathbb{C} : \det(\lambda I - T) = 0\} = \{1, -\tfrac{1}{2}\}$$

Since T is diagonalizable, $T_\lambda = \prod_{\zeta \in \Lambda_T \setminus \{\lambda\}} \frac{T - \zeta I}{\lambda - \zeta}$, yielding:

$$T_1 = \frac{T + \frac{1}{2} I}{1 + \frac{1}{2}} = \frac{1}{3} \begin{bmatrix} 2 & 1 \\ 2 & 1 \end{bmatrix} = |\mathbf{1}\rangle \langle \pi| \to \pi = (\tfrac{2}{3}, \tfrac{1}{3}) \text{ and}$$

$$T_{-\frac{1}{2}} = \frac{T - I}{-\frac{1}{2} - 1} = \frac{1}{3} \begin{bmatrix} 1 & -1 \\ -2 & 2 \end{bmatrix}.$$



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&= \delta[\tau]\, \frac{2}{3} + u[|\tau|-1] \left(\langle\pi|\, T^{(1)}\, |\mathbf{1}\rangle^2 + \left(-\tfrac{1}{2}\right)^{|\tau|-1} \langle\pi|\, T^{(1)} T_{-\frac{1}{2}} T^{(1)}\, |\mathbf{1}\rangle \right)
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&= \delta[\tau] \, \frac{2}{3} + u[|\tau| - 1] \left(\tfrac{4}{9} + \left(-\tfrac{1}{2} \right)^{|\tau|-1} \left(-\tfrac{1}{18} \right) \right)
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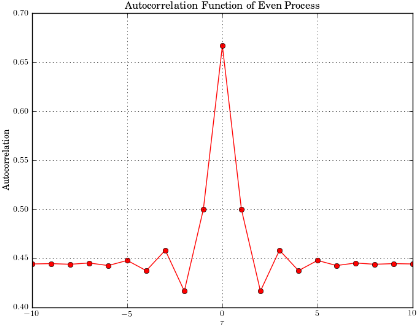
&= \delta[\tau]\,\frac{2}{3} + u[|\tau|-1]\tfrac{1}{9}\left(4 - \tfrac{1}{2}\left(-\tfrac{1}{2}\right)^{|\tau|-1}\right)
\end{aligned}
$$



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$$P_c(\omega) = \langle \pi | \, T^{(1)} \, | \mathbf{1} \rangle + 2 \sum_{\lambda \in \Lambda_T} \mathrm{Re} \frac{\langle \pi | \, T^{(1)} T_\lambda T^{(1)} \, | \mathbf{1} \rangle}{e^{i\omega} - \lambda}$$

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$$= \frac{2}{3} + 2 \left(\tfrac{4}{9} \mathrm{Re} \frac{1}{e^{i\omega} - 1} - \tfrac{1}{18} \mathrm{Re} \frac{1}{e^{i\omega} + \frac{1}{2}} \right)$$

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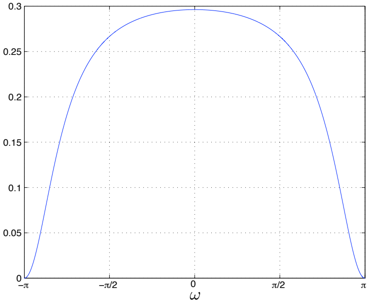

For chaotic crystals (polytypes), the power spectra of the stacking sequence given the alphabet of complex-valued structure factors is called the diffraction spectrum. And this is exactly what is measured with X-ray diffraction!

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Up next: Modes of information transduction; Exact complexity measures in closed form!