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Beyond Generalized Eigenvalues

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Notation

$C_{ab}(t)$	scalar correlation function $\in \mathbb{C}^{1\times 1}$
t	integer-spaced Euclidean time separations
$\boldsymbol{C}(t)$	matrix correlation function $\in \mathbb{C}^{N\times N}$
N	dimension of operator basis
a, b, n	operator indices $\in [1, N]$
L	exact polynomial order
K	assumed polynomial order
ℓ	index $\in [0, L-1]$ or $[0, K-1]$
k	index of states contributing to $\boldsymbol{C}(t)$
λ_k	$\exp(-E_k)$ energy of state contributing to $\boldsymbol{C}(t)$
z_{ak}	$\langle 0 \vert \mathcal{O}_a \vert k\rangle$ amplitude of state contributing to $\boldsymbol{C}(t)$

Correlation Function

$$\begin{aligned} C_{ab}(t) &= \sum_k \langle 0 \vert \mathcal{O}_a \vert k\rangle \exp(-E_k t) \left\langle k \middle\vert \mathcal{O}_b^\dagger \middle\vert 0 \right\rangle \\ &= z_{ak}\lambda_k^t z_{bk}^* = \boldsymbol{Z}\boldsymbol{\Lambda}^t\boldsymbol{Z}^\dagger \end{aligned}$$

We assume operator basis constructed so **C**(t) is Hermitian

Simple Effective Energy

$$\begin{aligned} C(t) &= [\lambda_{\text{eff}}(t,t_0)]^{t-t_0}\, C(t_0) \quad (t > t_0) \\ \implies & [\lambda_{\text{eff}}(t,t_0)]^{t-t_0} - [C(t_0)]^{-1}C(t) = 0 \\ \implies & E_{\text{eff}}(t,t_0) = -\frac{1}{t-t_0}\log\frac{C(t)}{C(t_0)} \end{aligned}$$

Generalized Eigenvalues

Extends simple effective mass to matrix-valued correlation functions

$$\det\left\{\boldsymbol{C}(t) - [\lambda_{\text{eff},k}(t,t_0)]^{t-t_0}\boldsymbol{C}(t_0)\right\} = 0$$

$$\implies \det\left\{[\lambda_{\text{eff},n}(t,t_0)]^{t-t_0}\boldsymbol{I} - [\boldsymbol{C}(t_0)]^{-1}\boldsymbol{C}(t)\right\} = 0$$

Reduces to finding eigenvalues provided $C(t_0)$ invertable.

Extending effective mass to matrices increases solution space 1 → N.

Prony's Method (1795)

Linear Prediction

$$\mathcal{P}_K(\lambda) = \prod_{k=1}^{K}(\lambda - \lambda_k) = \lambda^K + \sum_{\ell=0}^{K-1} p_\ell \lambda^\ell$$

$$\mathcal{P}_K(\lambda_k) = 0$$

$$\implies \lambda_k^K = -\sum_{\ell=0}^{K-1} p_\ell \lambda_k^\ell$$

Assuming only K states in C(t)

$$C(t) = -\sum_{\ell=0}^{K-1} p_\ell\, C(t-K+\ell)\ , \quad t \geq K$$

Prony's Method (1795) cont.

Solve for p_ℓ. $C_t \equiv C(t-t_0)$

$$\begin{bmatrix} C_K \\ C_{K+1} \\ \vdots \\ C_{2K-1} \end{bmatrix} = -\begin{bmatrix} C_0 & \cdots & C_{K-1} \\ C_1 & \cdots & C_K \\ \vdots & \ddots & \vdots \\ C_{K-1} & \cdots & C_{2K-2} \end{bmatrix} \begin{bmatrix} p_0 \\ p_1 \\ \vdots \\ p_{K-1} \end{bmatrix}$$

Find roots of polynomial λ_k. Alternatively, find eigenvalues of companion matrix.

$$\mathcal{C} = \begin{bmatrix} 0 & 0 & \cdots & 0 & -p_0 \\ 1 & 0 & \cdots & 0 & -p_1 \\ 0 & 1 & \ddots & \vdots & -p_2 \\ \vdots & \ddots & \ddots & 0 & \vdots \\ 0 & \cdots & 0 & 1 & -p_{K-1} \end{bmatrix}$$

After λ_k are known, amplitudes can be determined, just like simple case.

Extending effective mass from 2 times to 2K times increased solution size 1 → K.

Goal of This Work

Use N×N correlation matrices at 2·K equally-spaced times to find K·N effective energy solutions.

Block Prony Method (BPM)

Block Companion Matrix

$$\mathcal{C} = \begin{bmatrix} 0 & 0 & \cdots & 0 & -\boldsymbol{P}_0 \\ \boldsymbol{I} & 0 & \cdots & 0 & -\boldsymbol{P}_1 \\ 0 & \boldsymbol{I} & \ddots & \vdots & -\boldsymbol{P}_2 \\ \vdots & \ddots & \ddots & 0 & \vdots \\ 0 & \cdots & 0 & \boldsymbol{I} & -\boldsymbol{P}_{K-1} \end{bmatrix}$$

Assume K·N non-zero, non-degenerate eigenvalues λ_k. Let $\boldsymbol{v}_{k\ell}$ be size N blocks of kth eigenvector of $\mathcal{C}$, satisfying

$$\begin{aligned} \lambda_k \boldsymbol{v}_{k,0} &= -\boldsymbol{P}_0 \boldsymbol{v}_{k,K-1} \\ \lambda_k \boldsymbol{v}_{k,\ell} &= \boldsymbol{v}_{k,\ell-1} - \boldsymbol{P}_\ell \boldsymbol{v}_{k,K-1} \end{aligned}$$

After substitution

$$\lambda_k^K \boldsymbol{v}_{k,K-1} = \left(-\sum_{\ell=0}^{K-1}\lambda_k^\ell \boldsymbol{P}_\ell\right)\boldsymbol{v}_{k,K-1}$$

Block Prony Method (BPM) cont

Let $\boldsymbol{w}_\ell$ be size N blocks of any normalizable vector $\boldsymbol{w}$ in eigenspace of $\mathcal{C}$

$$\boldsymbol{C}_t \boldsymbol{w}_{K-1} = -\sum_{\ell=0}^{K-1}\boldsymbol{C}_{t-K+\ell}\,\boldsymbol{P}_\ell\,\boldsymbol{w}_{K-1}\ , \quad t \geq K$$

Solve for $\mathbf{P}_\ell$. $\mathbf{C}_t \equiv \mathbf{C}(t-t_0)$

$$\begin{bmatrix} \boldsymbol{C}_K \\ \boldsymbol{C}_{K+1} \\ \vdots \\ \boldsymbol{C}_{2K-1} \end{bmatrix} = -\begin{bmatrix} \boldsymbol{C}_0 & \cdots & \boldsymbol{C}_{K-1} \\ \boldsymbol{C}_1 & \cdots & \boldsymbol{C}_K \\ \vdots & \ddots & \vdots \\ \boldsymbol{C}_{K-1} & \cdots & \boldsymbol{C}_{2K-2} \end{bmatrix} \begin{bmatrix} \boldsymbol{P}_0 \\ \boldsymbol{P}_1 \\ \vdots \\ \boldsymbol{P}_{K-1} \end{bmatrix}$$

Then K·N eigenvalues of block companion $\mathcal{C}$ matrix are effective energies.

Effective Amplitudes

Once λ_k are known, challenge is to solve bilinear system of equations (BLS)

$$C_{ab}(t) = \sum_{k=1}^{KN} z_{ak}\lambda_k^t z_{bk}^*$$

No general method to solve BLS is known. See Johnson *et al*.

Equal number of equations and unknowns.

$$C_{ab}(t):\ 2K\frac{N(N+1)}{2}\ , \quad \lambda_k:\ KN\ , \quad z_{ak}: N(KN)$$

Exact solution should be possible up to signs: $z_{ak} \to -z_{ak}$ for any k.

For now, we recommend searching for zero residual solutions using non-linear least squares minimization.

References for Further Reading

Fleming, Cohen, Lin and Pereyra, arXiv:0903.2314 [hep-lat]

Gohberg, Lancaster and Rodman, *Matrix Polynomials*, SIAM 2009.

Johnson, Šmigoc and Yang, arXiv:1303.4988 [math.RA]

Cushman and Fleming, arXiv:1912.08205 [hep-lat]

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