Lanczos for spectroscopy

LaMET 2024
Aug 13, 2024
University of Maryland

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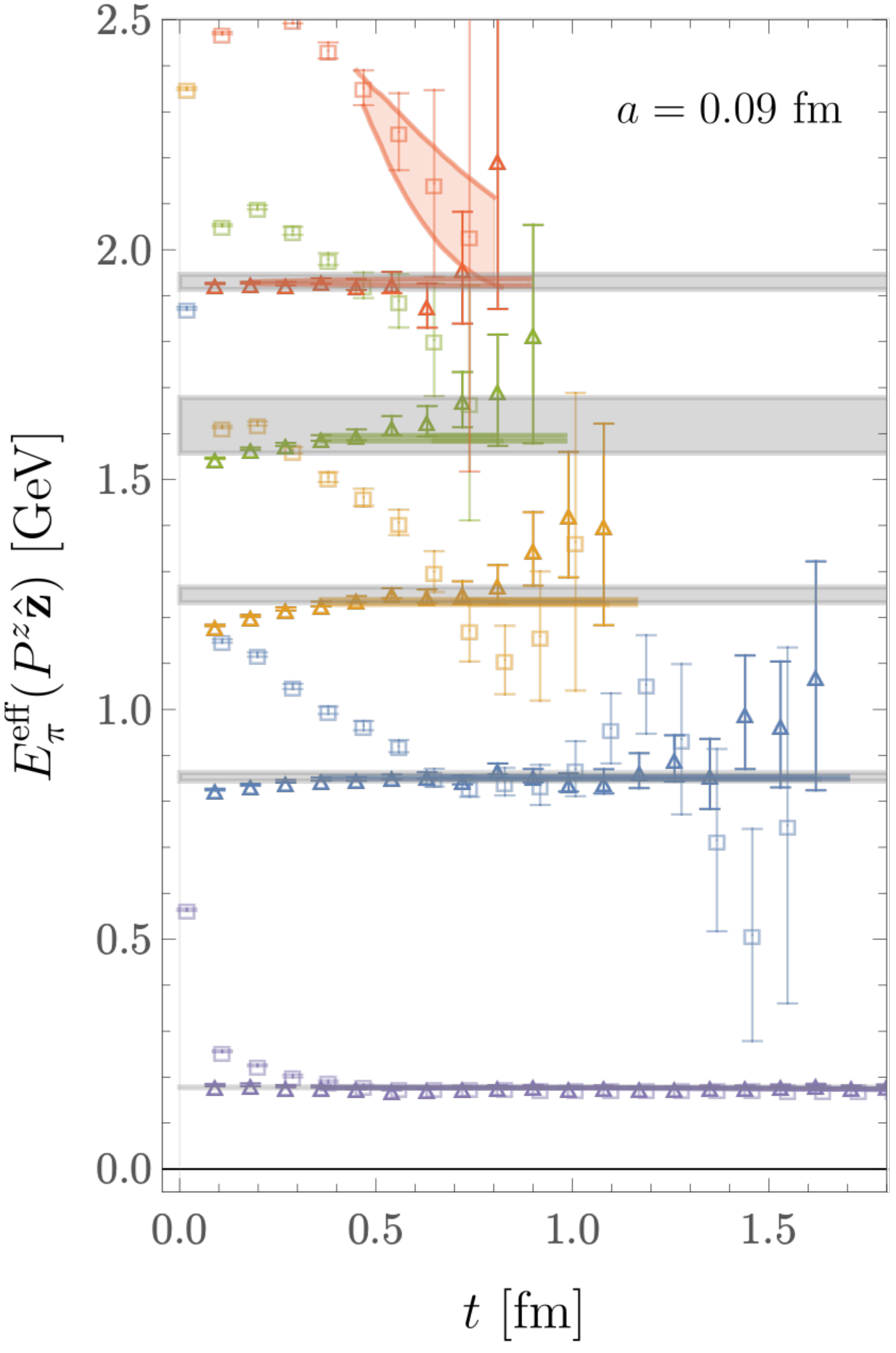
Boosted states are noisy



Avkhadiev, Shanahan, MW, Zhao, PRL 132 (2024)

Exponential signal-to-noise degradation common to all large-momentum correlation functions used for LaMET

e.g. pion state

$$\text{signal} \sim e^{-E(\mathbf{P})t}$$

$$\text{variance} \sim e^{-2m_\pi t}$$

$$\frac{\text{signal}}{\text{noise}} \sim e^{-[E(\mathbf{P})-m_\pi]t}$$

Outline

- Spectroscopy and the transfer matrix
- Lanczos spectroscopy algorithm
- “Spurious eigenvalues”
- Proof-of-principle demonstrations

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- **Spectroscopy and the transfer matrix**
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Spectroscopy = finding eigenvalues

Lattice theories do not have continuous time translation symmetry defining Hamiltonian

$$\mathcal{O}(t) = e^{-Ht}\mathcal{O}e^{Ht}$$ ✗

Discrete time translation symmetry enables definition of transfer matrix T

$$\mathcal{O}(ka) = T^k\mathcal{O}(T^{-1})^k$$ ✓

Energy spectrum = - ln (spectrum of eigenvalues of T)

$$T\big|n\big\rangle = \big|n\big\rangle\lambda_n \qquad E_n = -\ln\lambda_n$$

Correlation functions are matrix elements of powers of T

$$C(t) \equiv \langle\psi(t)\psi^\dagger(0)\rangle = \left\langle\psi\right|T^{t/a}\left|\psi\right\rangle + \ldots$$

Hilbert space & the Schrodinger picture

Interpolator excites the starting state

$$\bar{\psi}\,|\Omega\rangle = |\psi\rangle = \sum_k \langle k|\psi\rangle\,|k\rangle \equiv \sum_k Z_k|k\rangle$$

Hermitian transfer matrix

$$T = T^\dagger = \sum_k |k\rangle\,\lambda_k\,\langle k|$$

where $\lambda_k = e^{-E_k t}$

Euclidean time evolution

$$T^t|\psi\rangle = \sum_k Z_k\,e^{-E_k t}|k\rangle$$

$$\rightarrow \quad Z_0 e^{-E_0 t}|0\rangle + (\mathrm{ESC})$$

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$$\to \quad Z_0 e^{-E_0 t}|0\rangle + (\mathrm{ESC})$$

No access to states/operators, but can compute correlators:

$$C(t) = \langle\psi|T^t|\psi\rangle$$

$$= \sum_k |Z_k|^2\,\lambda_k^t$$

The power iteration algorithm

Apply m hits of T to purify ground state

$$|0\rangle \approx \left|b^{(m)}\right\rangle = \frac{T^m|\psi\rangle}{||T^m|\psi\rangle||} = \frac{T^m}{\sqrt{\langle\psi|T^{2m}|\psi\rangle}}$$

Approximate $\lambda_0 = \langle 0|T|0\rangle$ as

$$\lambda_0^{(m)} = \left\langle b^{(m)}|T|b^{(m)}\right\rangle = \frac{\langle\psi|T^{2m+1}|\psi\rangle}{\langle\psi|T^{2m}|\psi\rangle}$$

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Recover usual effective energy:

$$E^{\text{eff}}(2t) = \log\lambda_0^{(2t)} = \log\frac{C(2t+1)}{C(2t)}$$

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Lanczos and the transfer matrix

- Standard effective mass = "power-iteration algorithm" for finding eigenvalues

$$\left|b^{(t)}\right\rangle \propto T^t|\psi\rangle \quad \Rightarrow \quad \log\left\langle b^{(t)}\middle|T\middle|b^{(t)}\right\rangle = \log\frac{C(2t+1)}{C(2t)} = E^{\text{eff}}(2t)$$

von Mises and Pollaczek-Geiringer, Zeitschrift Angewandte Mathematik und Mechanik 9, 58 (1929)

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- Modern computational linear algebra uses more sophisticated methods, e.g.

Lanczos algorithm

Lanczos, J. Res. Natl. Bur. Stand. B 45, 255 (1950)

Applied to LQCD since at least Barbour et al (1984)

$$|v_j\rangle \propto [T - T^{(m)}]|v_{j-1}\rangle$$

$$T^{(m)}_{ij} = \langle v_i|T|v_j\rangle \quad \Rightarrow \quad E^{(m)}_k = -\ln\lambda^{(m)}_k$$

- Exponentially faster convergence for systems with small gaps $\delta = a(E_1 - E_0)$

Kaniel, Mathematics of Computation 20, 369 (1966)

Paige, PhD thesis 1971

Saad, SIAM 17 (1980)

$$\left|E_0 - E_0^{(m)}\right| \propto e^{-4m\sqrt{\delta}} \ll \left|E_0 - E^{\text{eff}}(2m)\right| \propto e^{-2m\delta}$$

The residual bound

- Lanczos approximation error after finite number of iterations directly computable:

$$\min_{\lambda \in \{\lambda_n\}} |\lambda_k^{(m)} - \lambda| \leq |\beta_{m+1}\, s_{mk}^{(m)}|$$

Eigenvectors of $T^{(m)}$

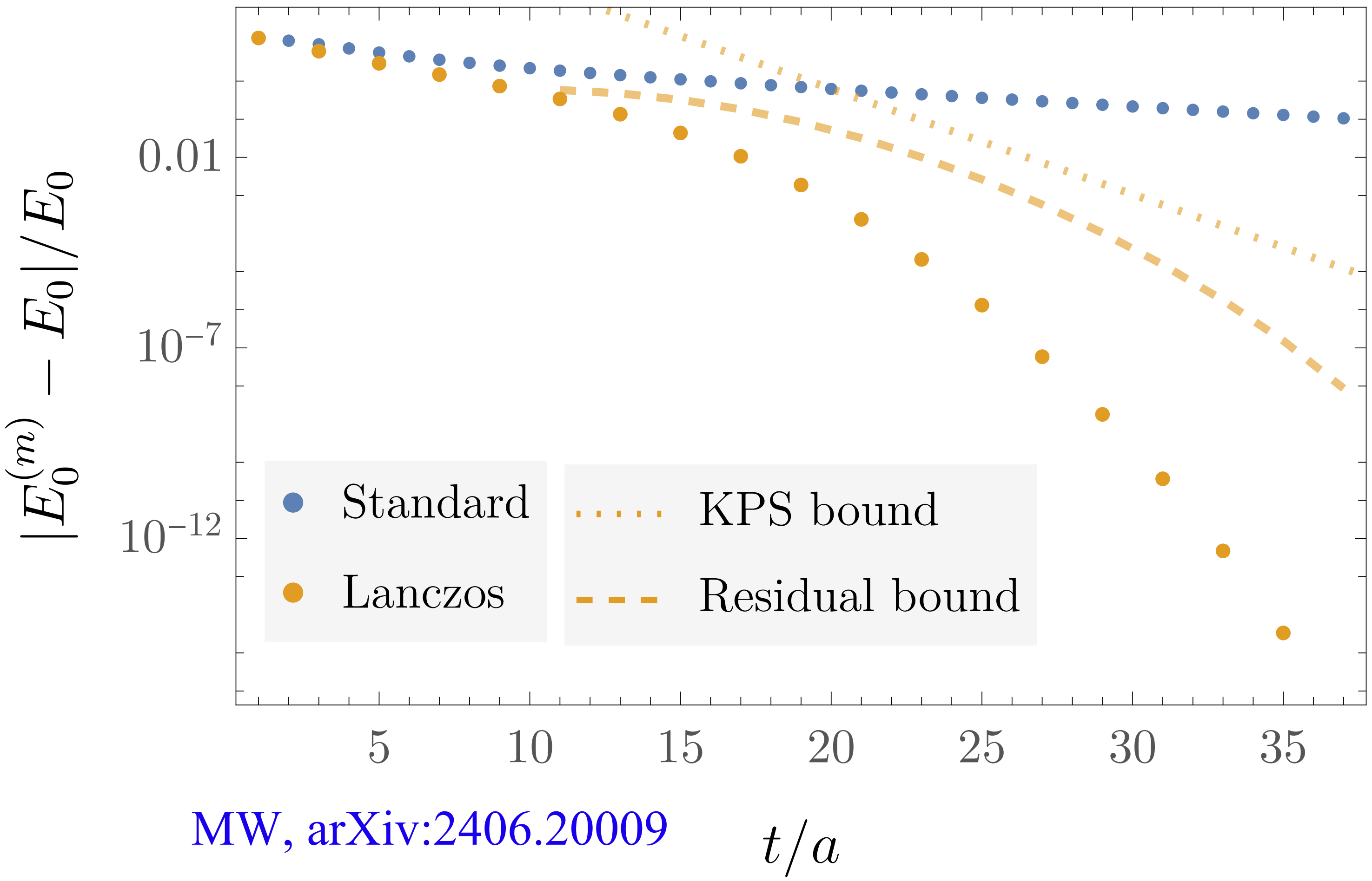
Matrix element $T^{(m)}_{m(m+1)}$

Paige, PhD thesis 1971

Rigorous quantification of excited-state effects!

But the LQCD transfer matrix is infinite-dimensional….

- Applying Lanczos feasible by computing matrix elements $T_{ij}^{(m)}$ recursively
- Faster convergence evident in studies of toy data



MW, arXiv:2406.20009

Lanczos in Hilbert space

Start:

$$|v_1\rangle = \frac{|\psi\rangle}{\sqrt{\langle\psi|\psi\rangle}} = \frac{|\psi\rangle}{\sqrt{C(0)}}$$

$$\alpha_1 = \langle v_1|T|v_1\rangle = \frac{C(1)}{C(0)}$$

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Iterate:

1. Apply T and orthogonalize
   $$|\tilde{v}_{j+1}\rangle = (T - \alpha_j)|v_j\rangle + \beta_j|v_{j-1}\rangle$$
2. Normalize & compute α
   $$\beta_{j+1}^2 = \langle\tilde{v}_{j+1}|\tilde{v}_{j+1}\rangle$$
   $$|v_{j+1}\rangle = \frac{1}{\beta_{j+1}}|\tilde{v}_{j=1}\rangle$$
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After m iterations:

Lanczos vectors $|v_j\rangle$ for $j = 1, \dots, m$

$$\langle v_i|v_j\rangle = \delta_{ij}$$

T in Lanczos vector basis:

$$T_{ij}^{(m)} = \langle v_i|T|v_j\rangle = \begin{bmatrix} \alpha_1 & \beta_2 & & & 0 \\ \beta_2 & \alpha_2 & \beta_3 & & \\ & \beta_3 & \alpha_3 & \ddots & \\ & & \ddots & \ddots & \beta_m \\ 0 & & & \beta_m & \alpha_m \end{bmatrix}$$

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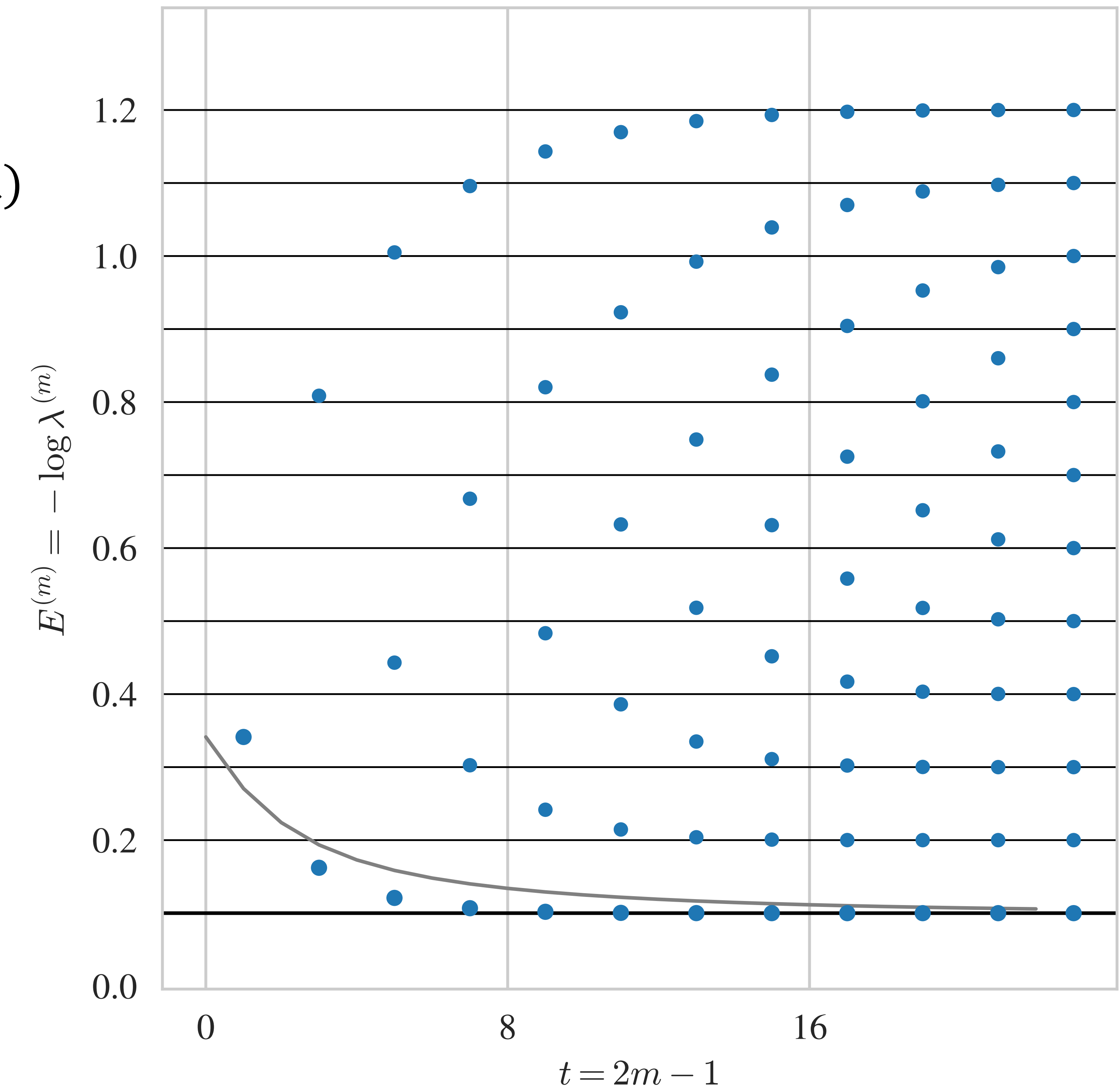
Can compute from $C(t) = \langle\psi|T^t|\psi\rangle$!
(via a recursion relation)

Diagonalizing T

$$T_{ij}^{(m)} = \sum_k s_{ik}^{(m)} \lambda_k^{(m)} (s^{-1})_{kj}^{(m)}$$

Ritz value $\approx e^{-E_k t}$



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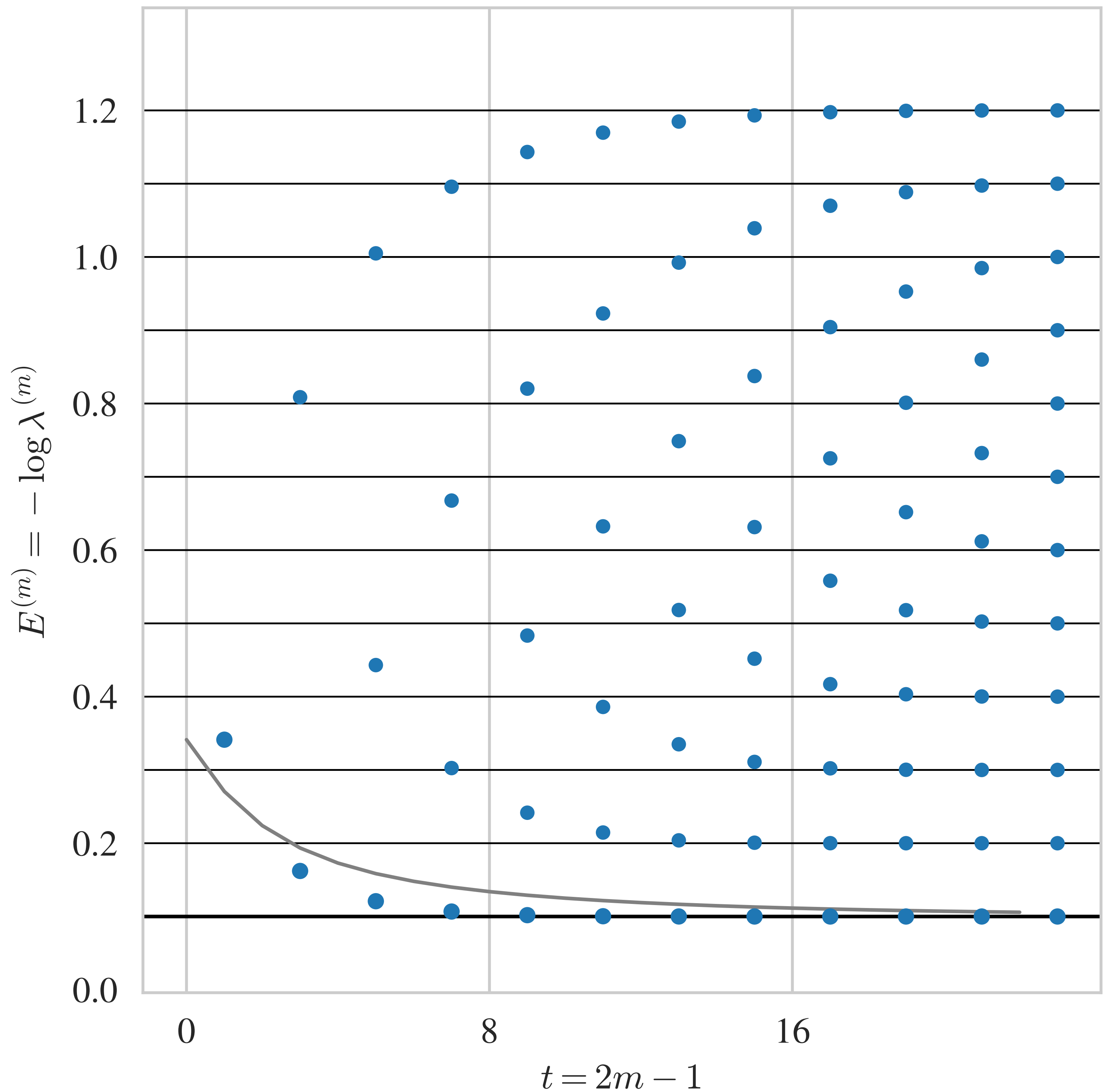
↑ Over all true eigenstates

↑ Computable from $C(t)$

Note: eigenvectors converge at same rate as eigenvalues! (Kaniel-Page-Saad)



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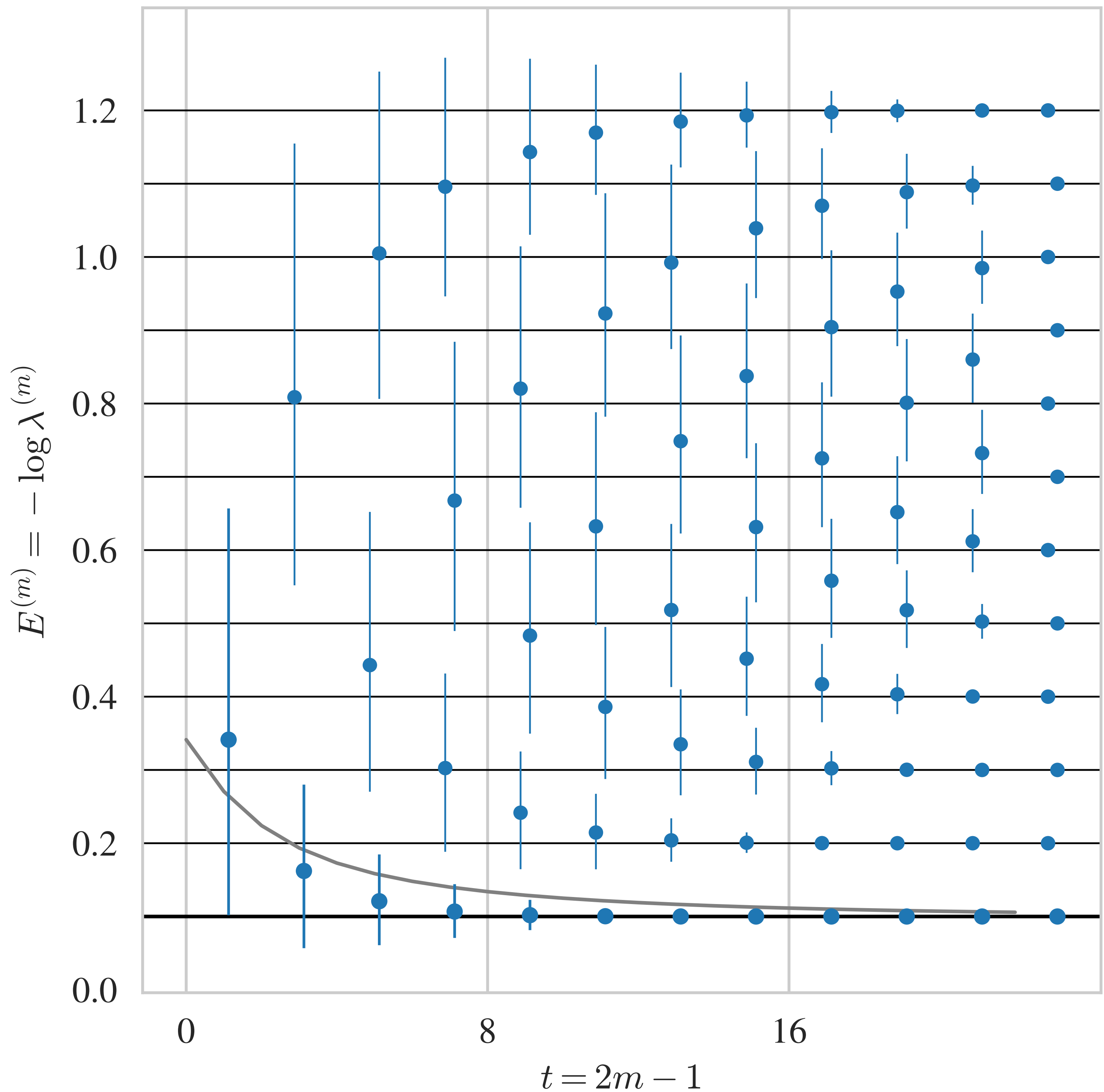

Will noise destroy Lanczos?

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- No

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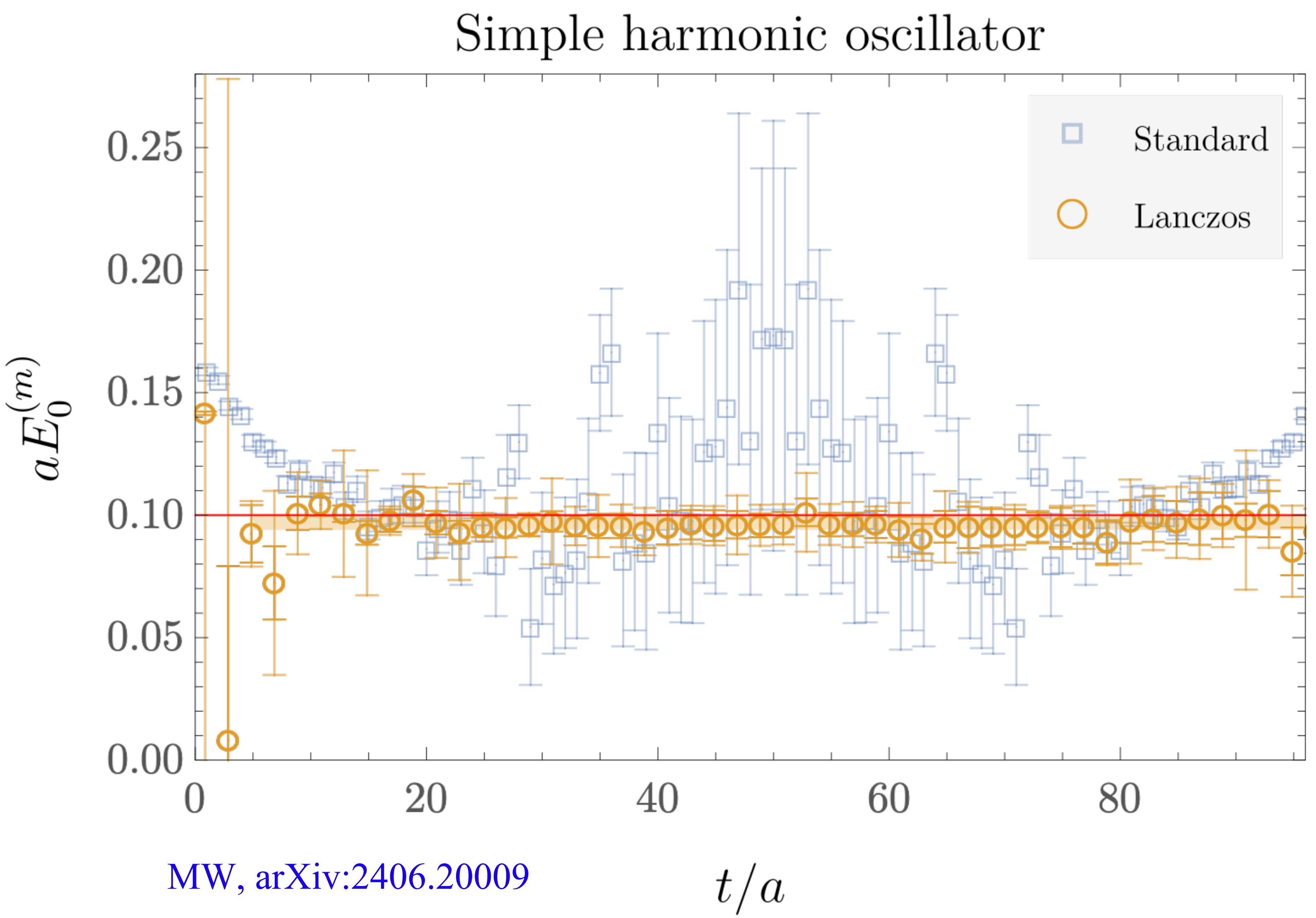
- Lanczos is surprisingly robust to large-time correlation function noise



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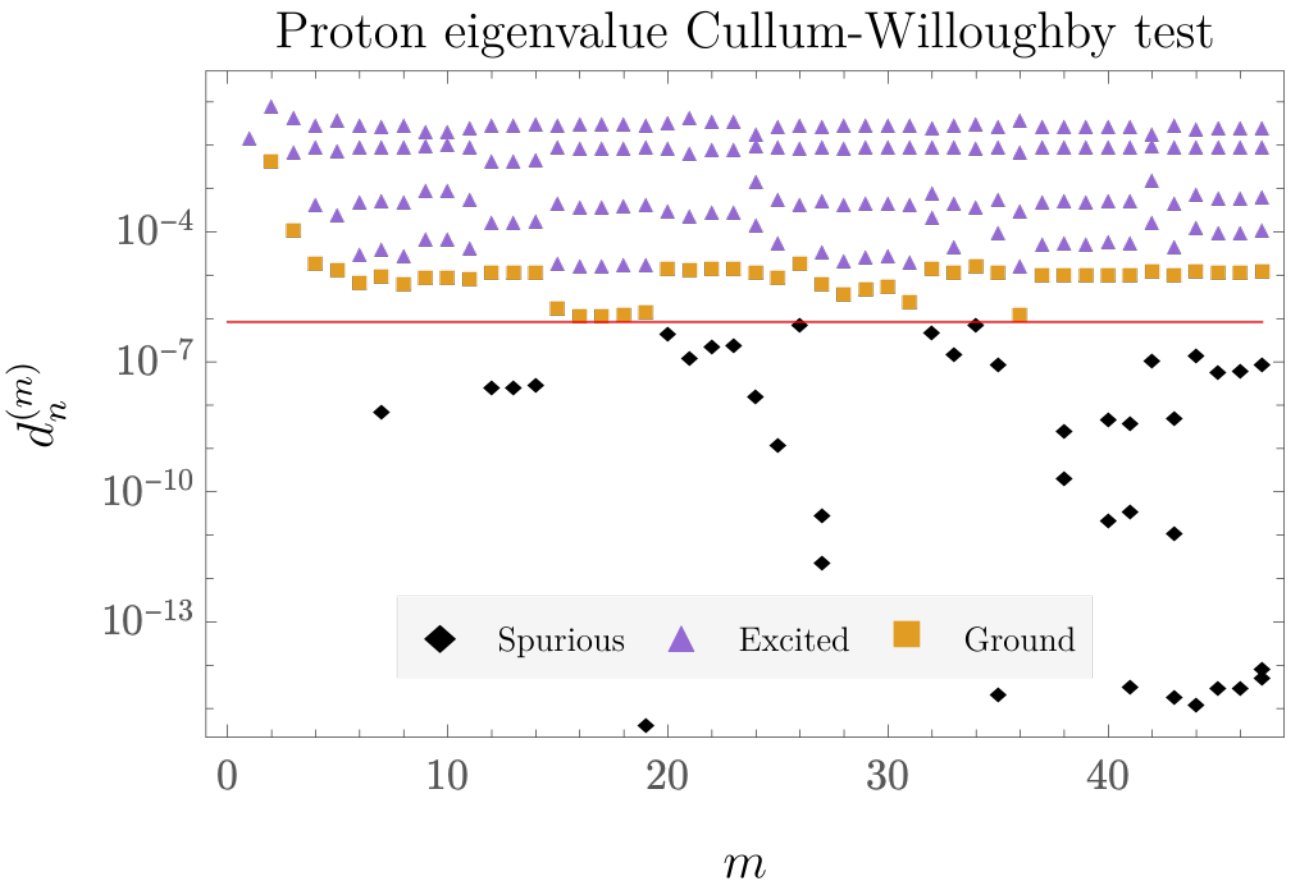
- **“Spurious eigenvalues”**



- Proof-of-principle demonstrations

Spurious eigenvalues

Example:

Luscher-Weisz gauge action

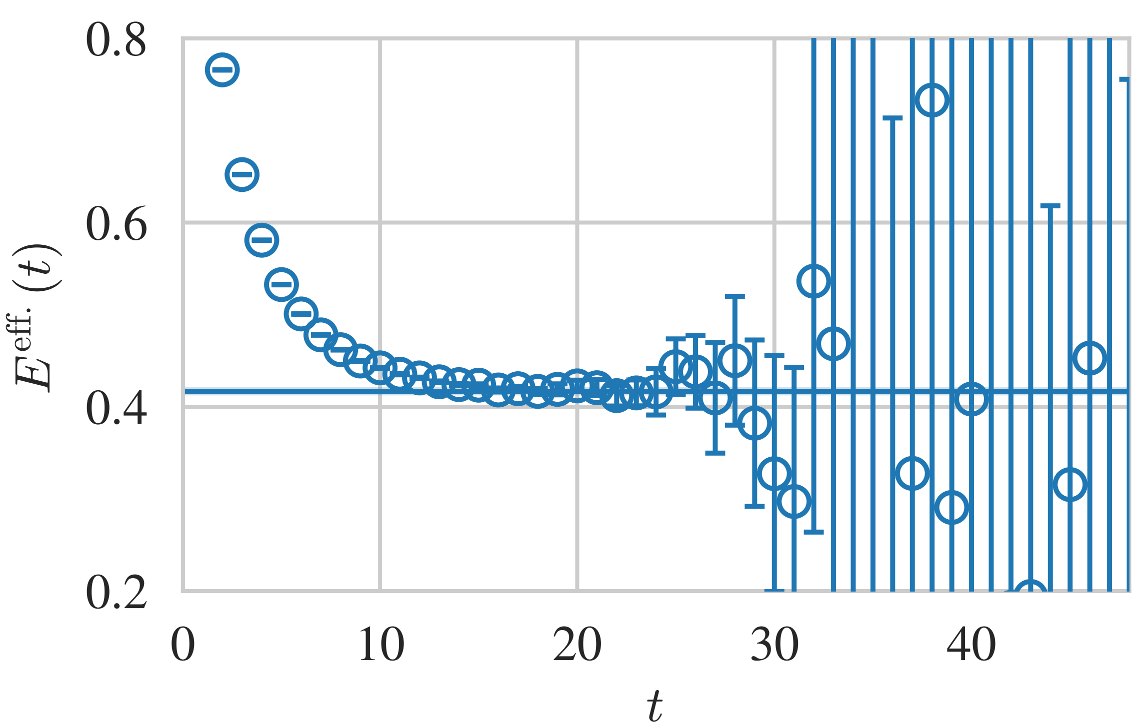
2+1 stout-smeared clover fermions

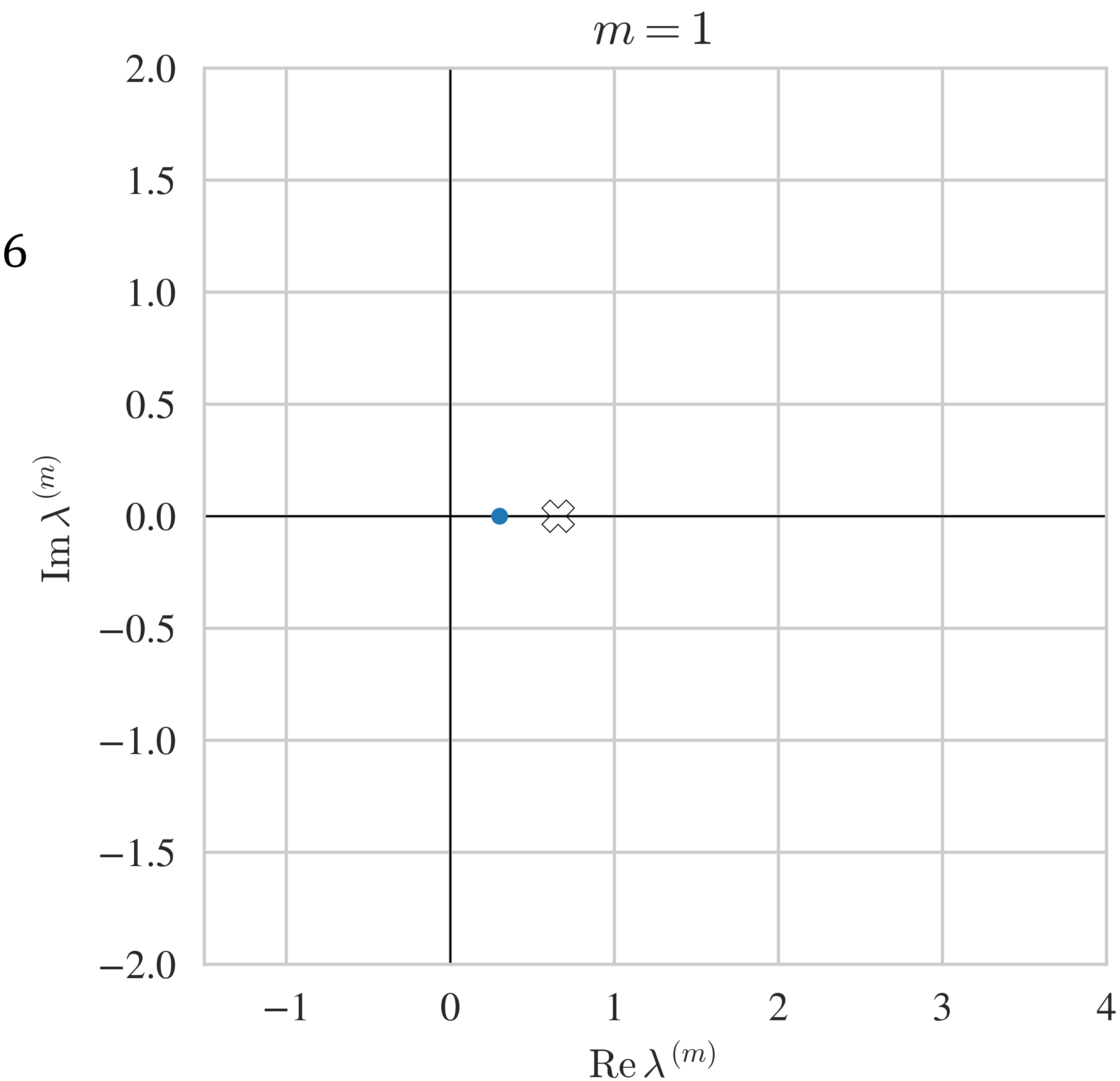
$M_\pi \approx 170$ MeV $\quad a \approx 0.09$ fm $\quad 48^3 \times 96$

Nucleon $\quad \chi \sim (u\, C\, \gamma_5\, d)\, u$

Quarks smeared to $r = 4.5$

✠ ~ known λ_0 from multi-state fits





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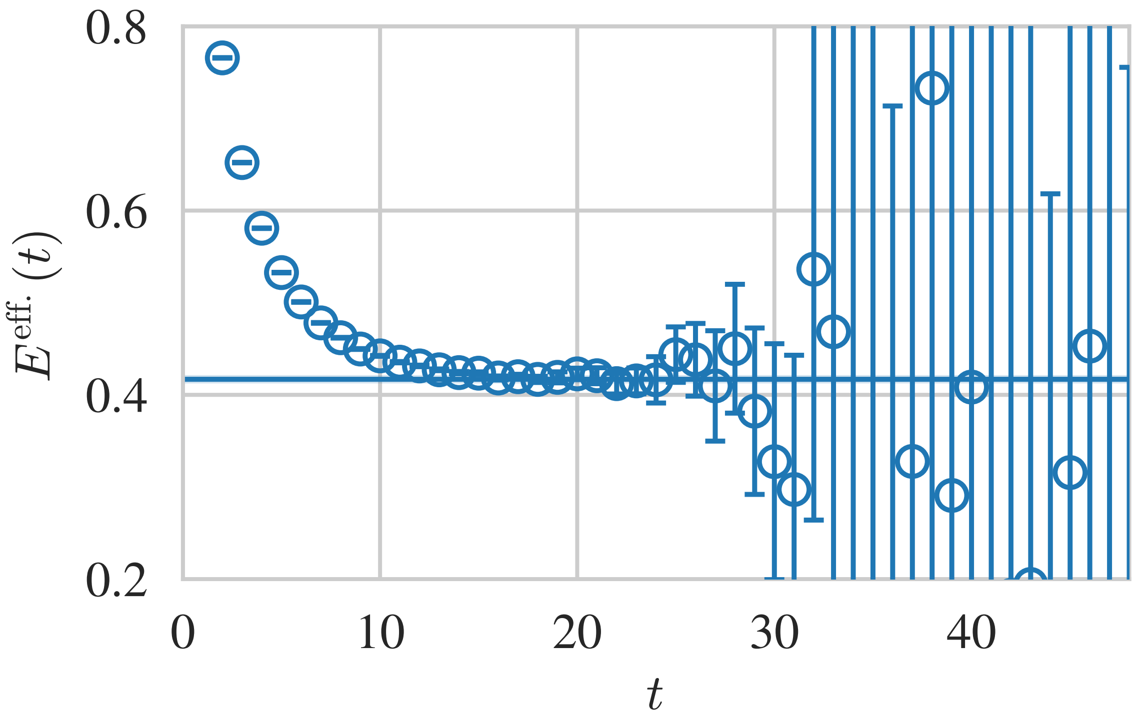

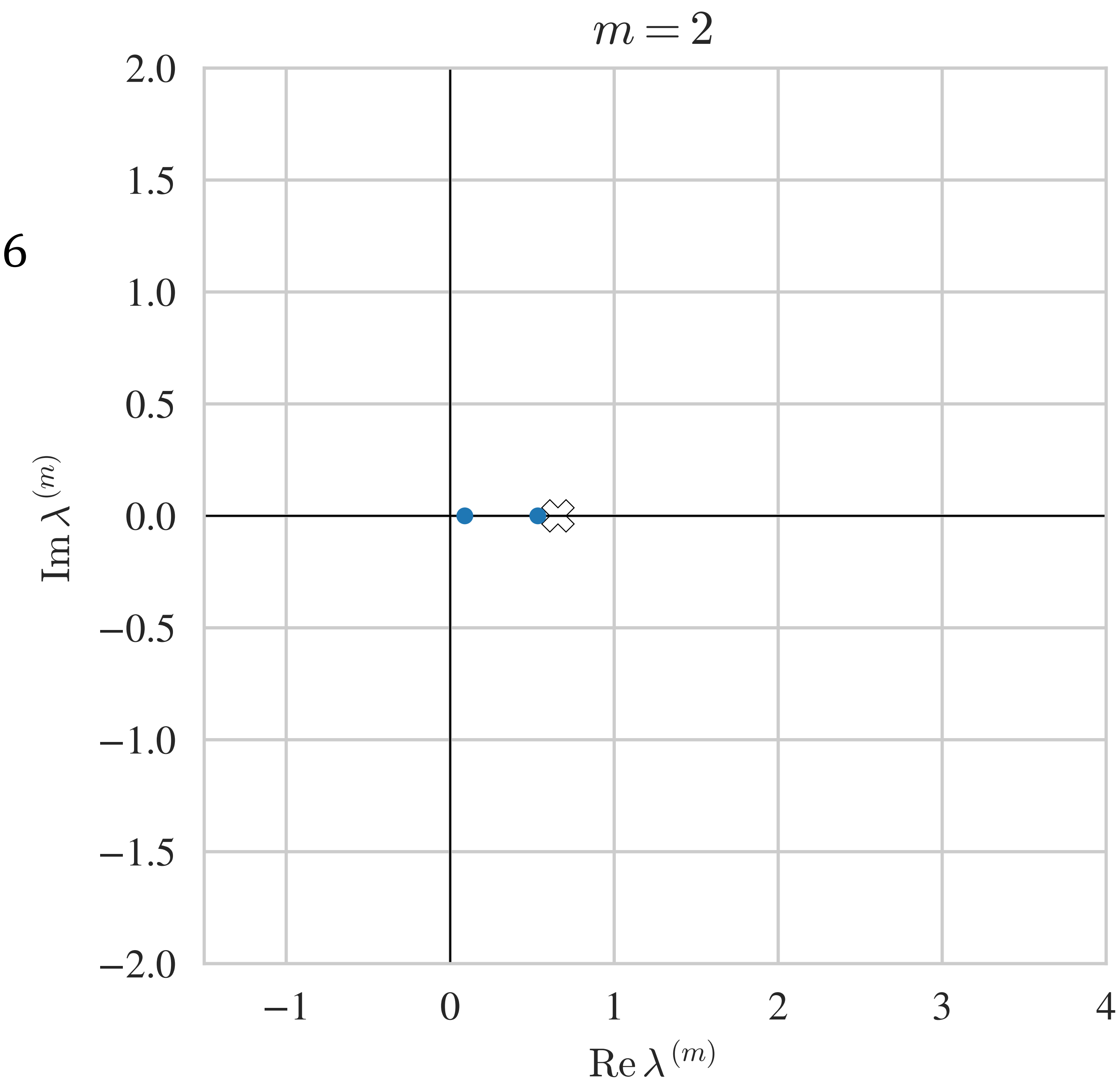

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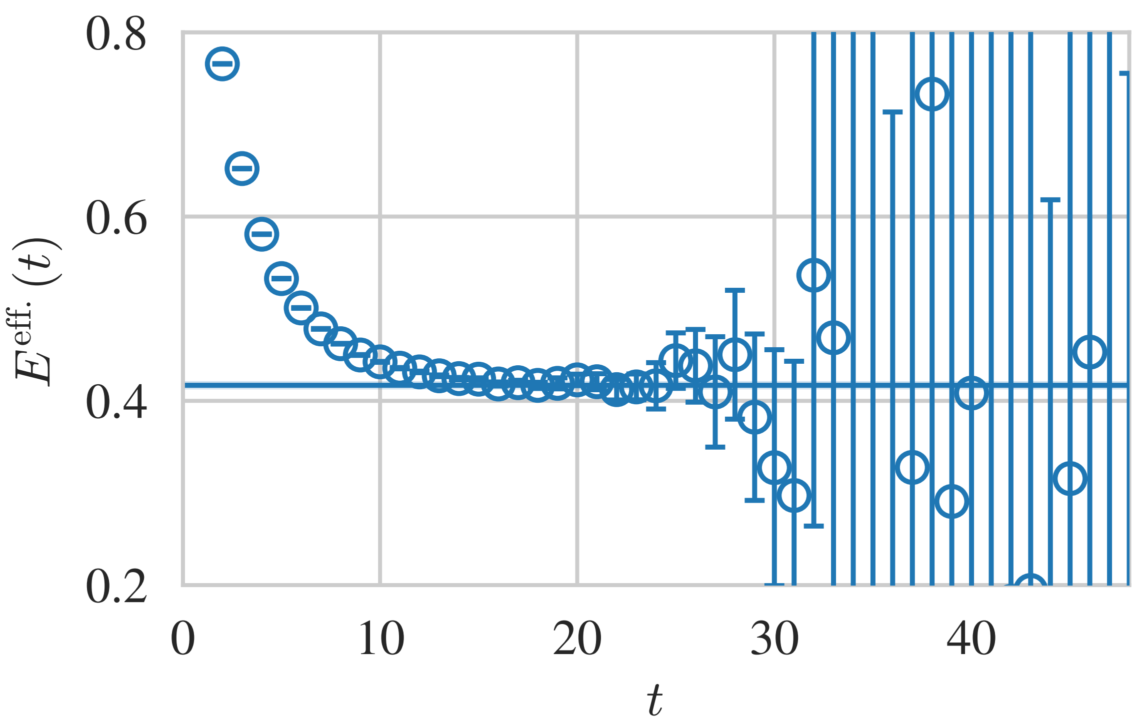

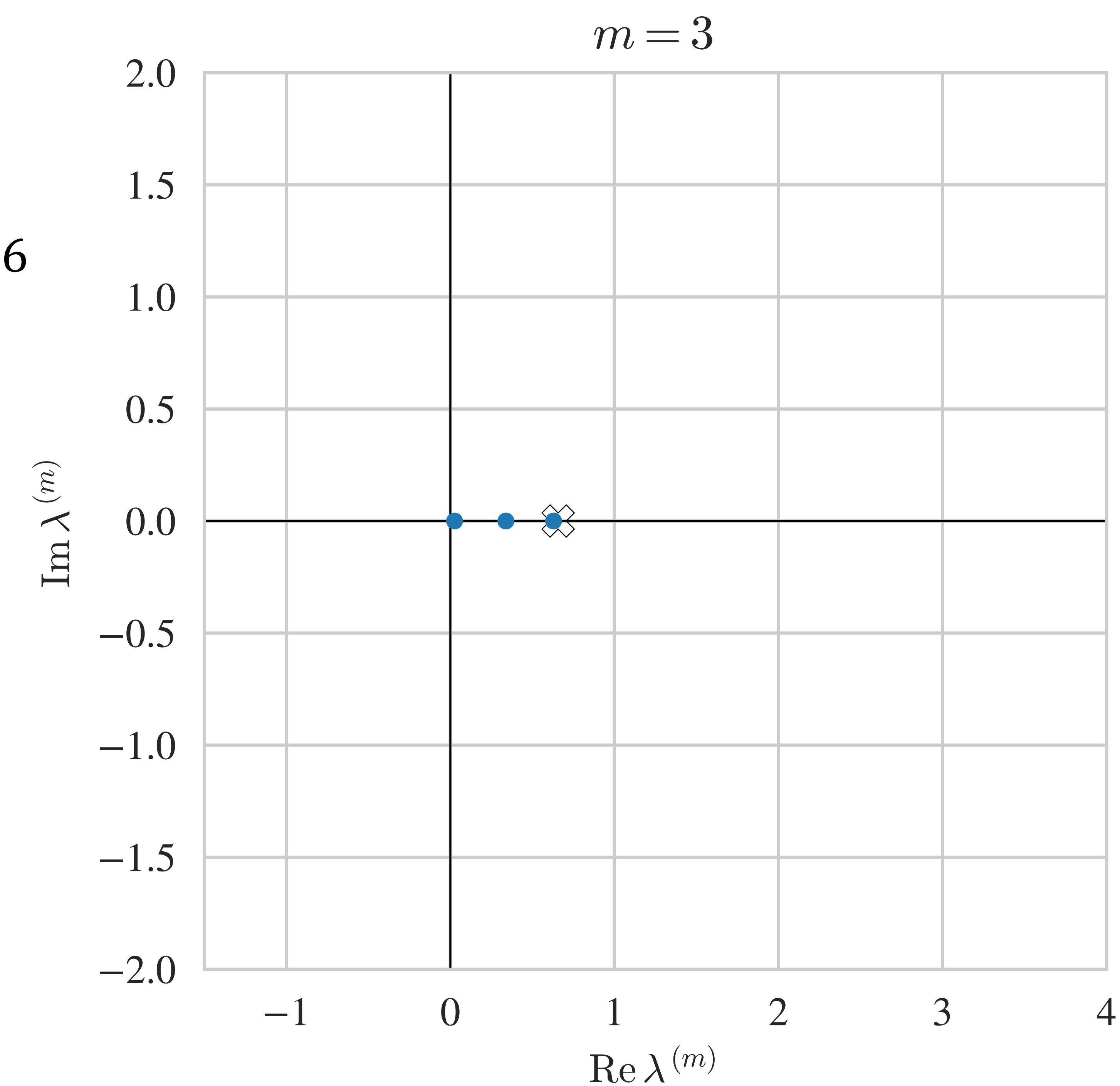

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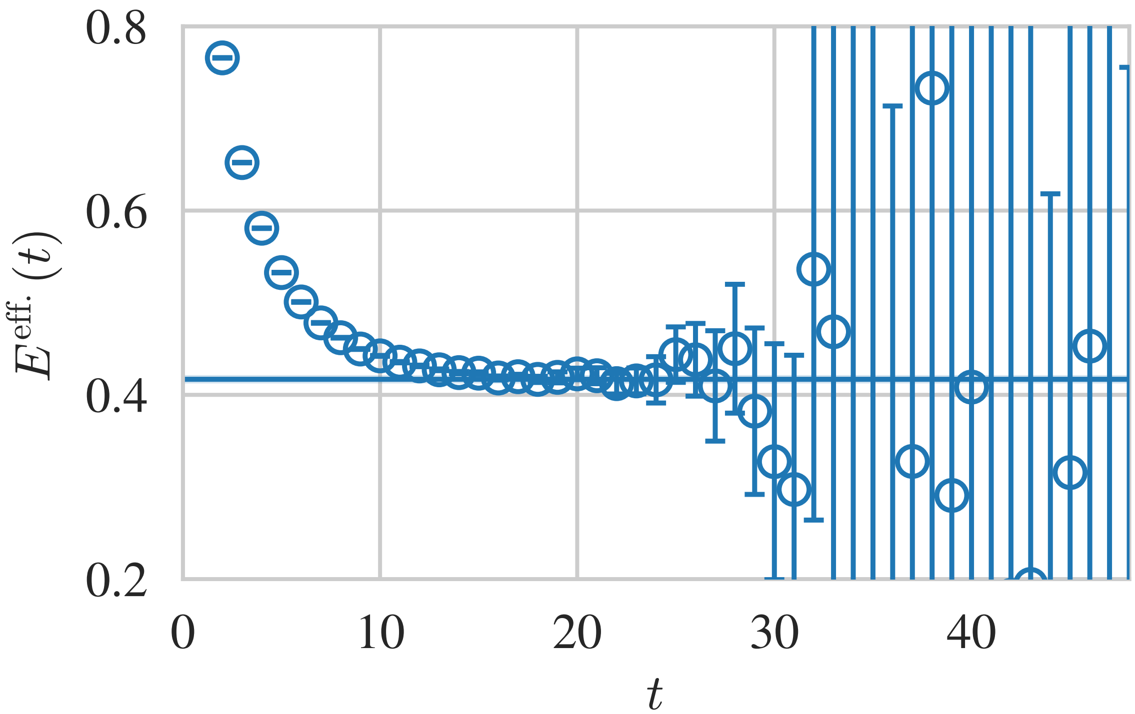

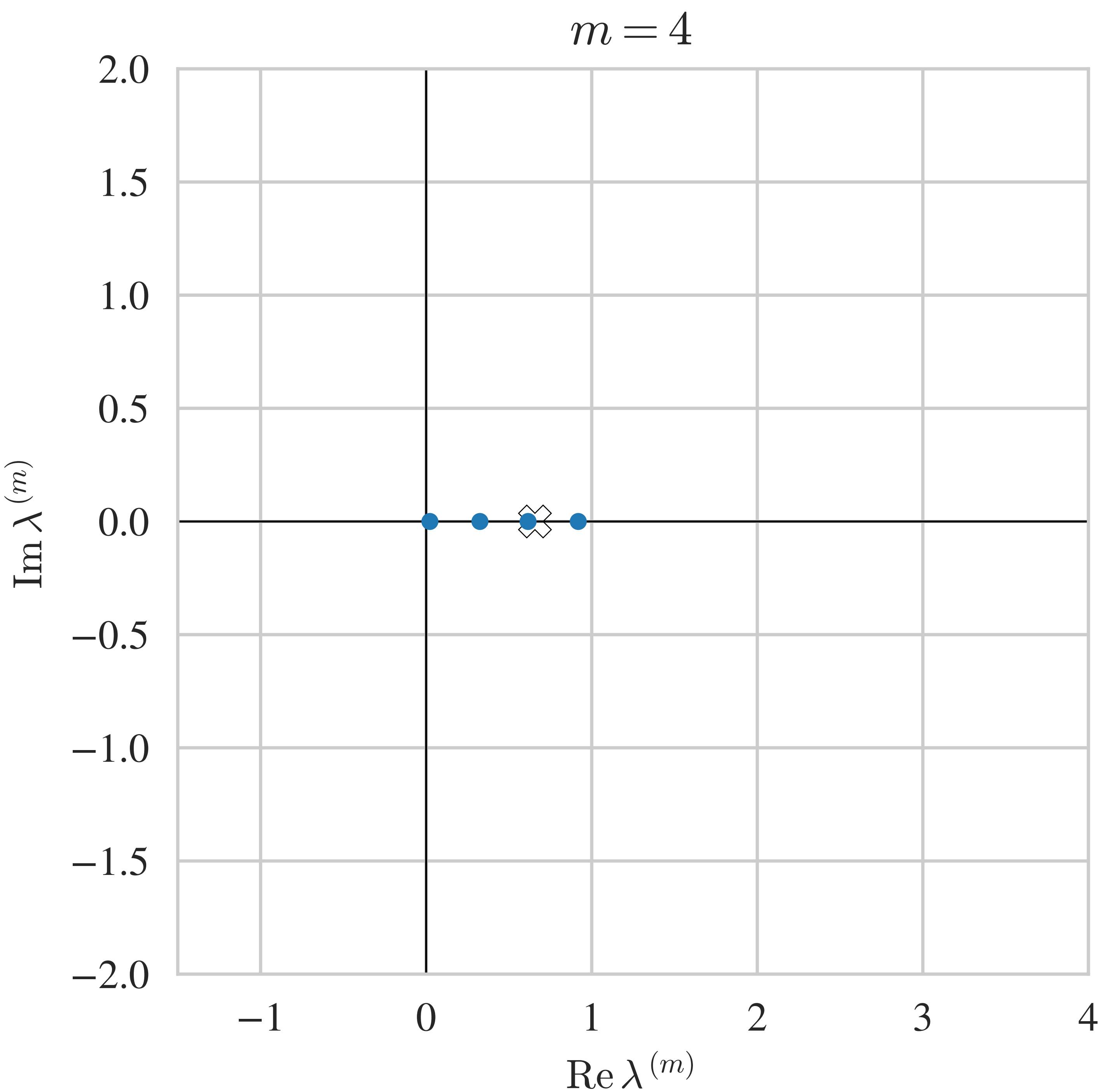

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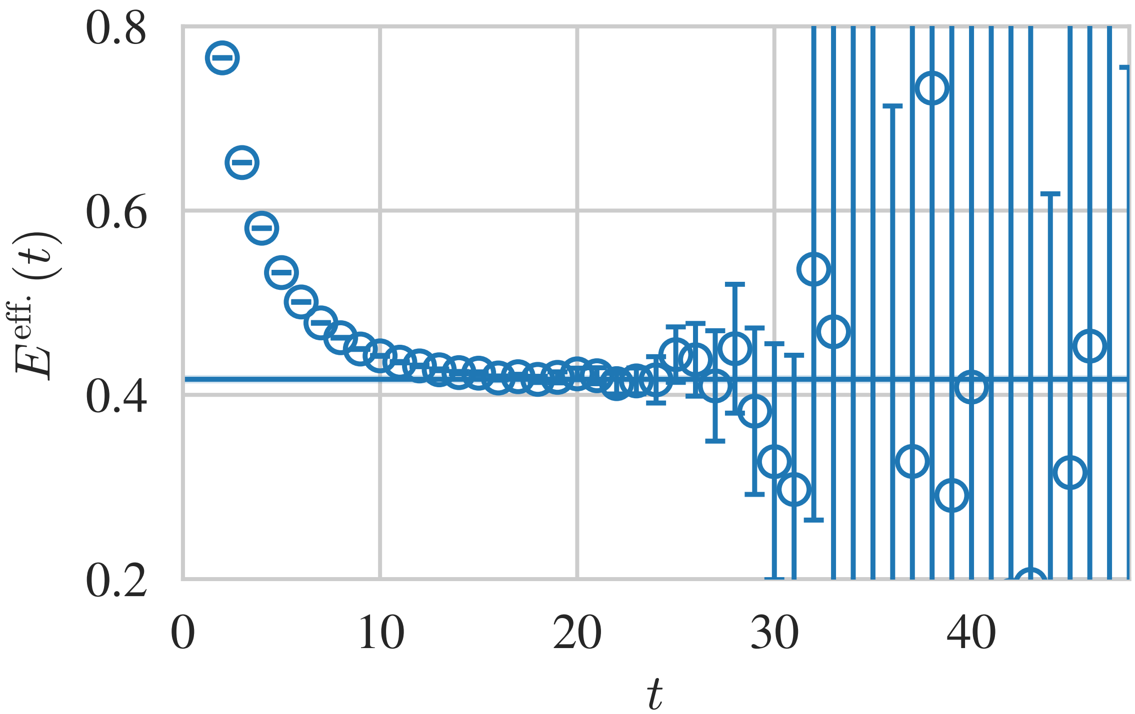

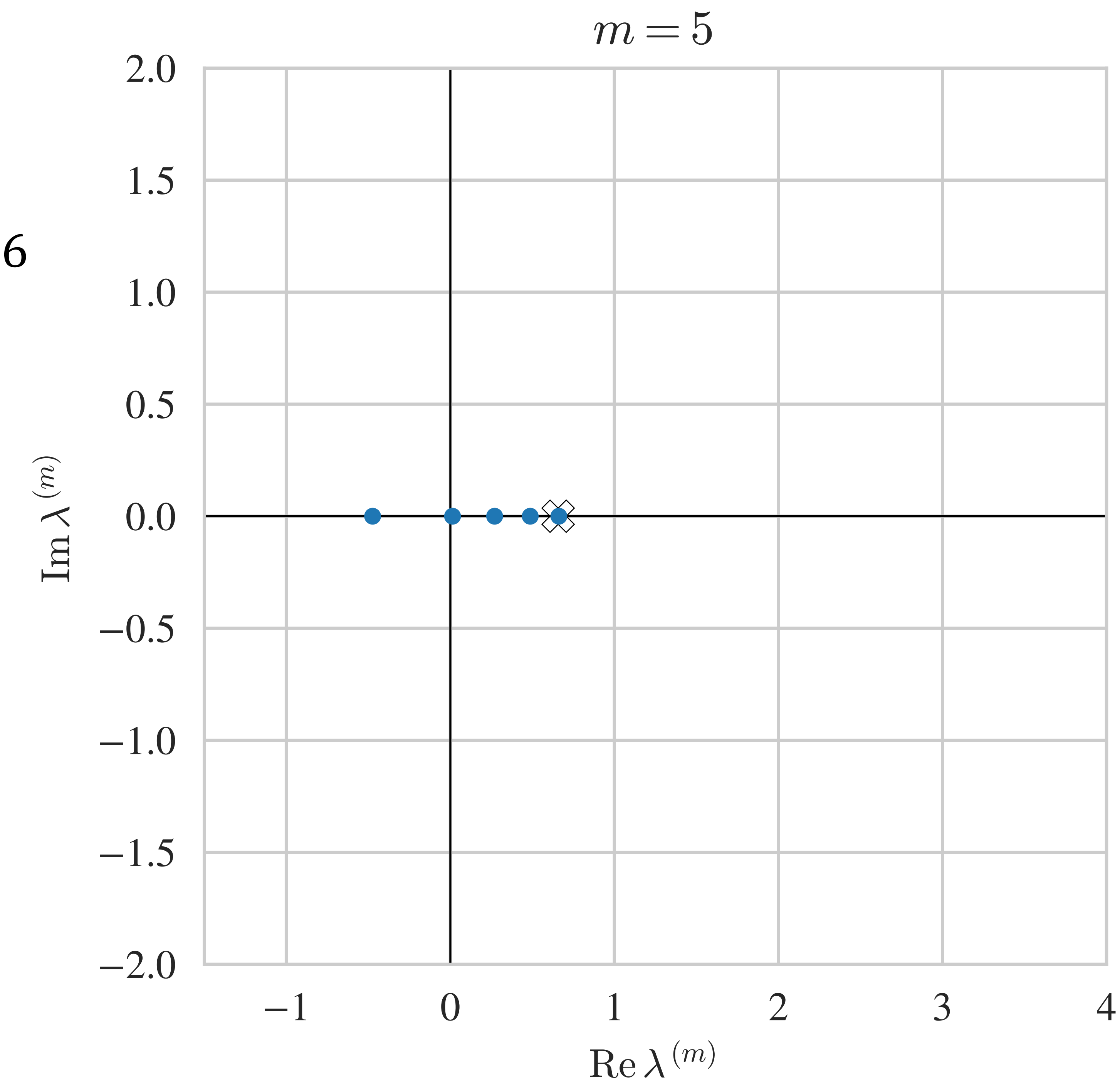

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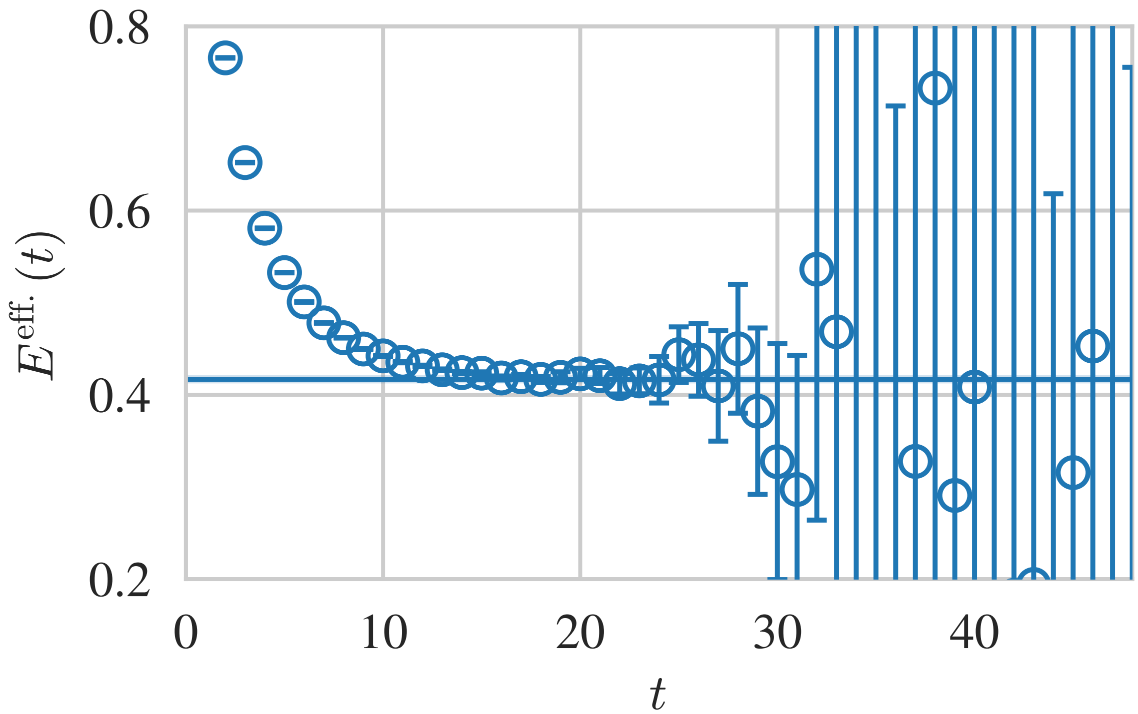

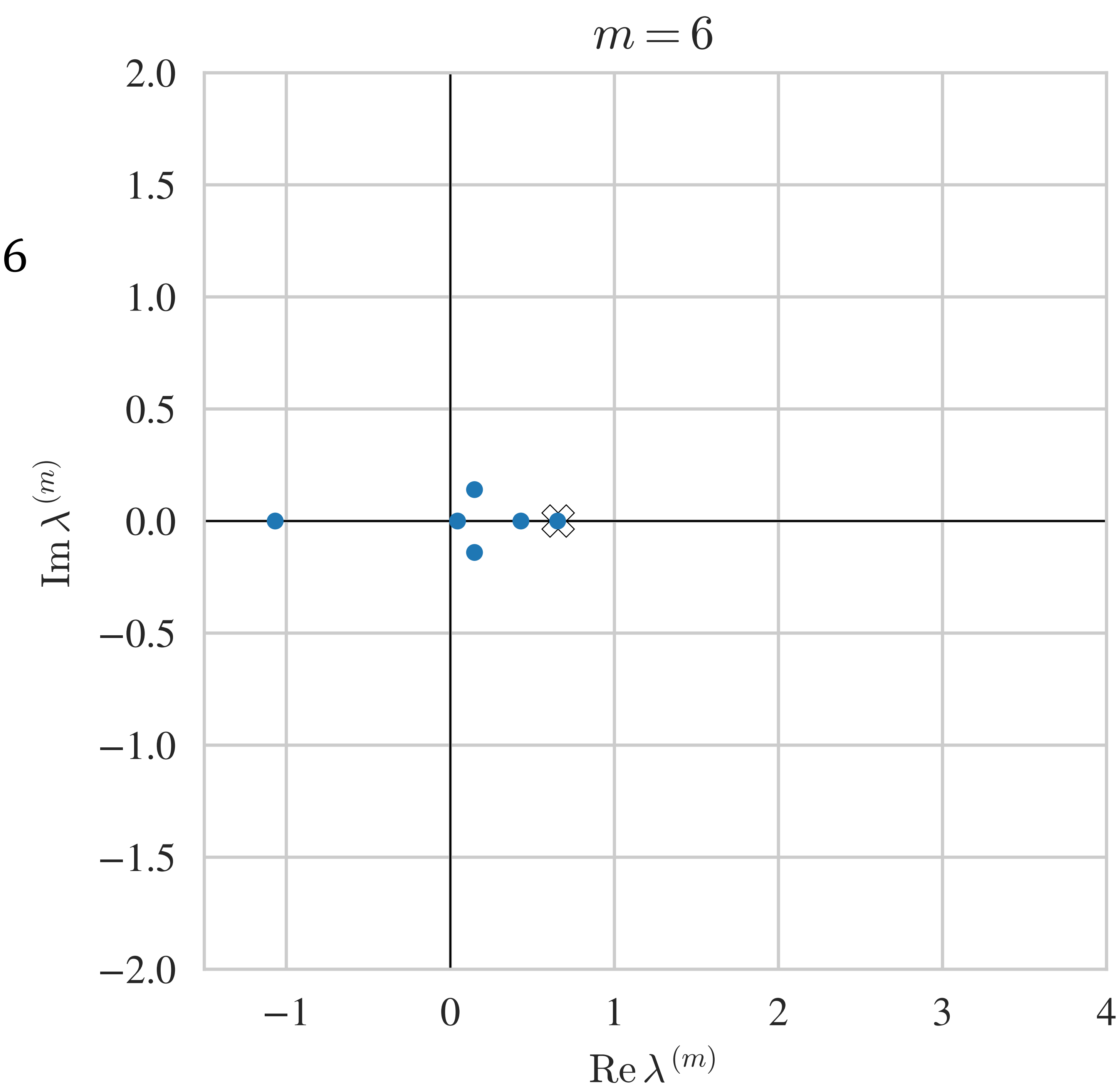

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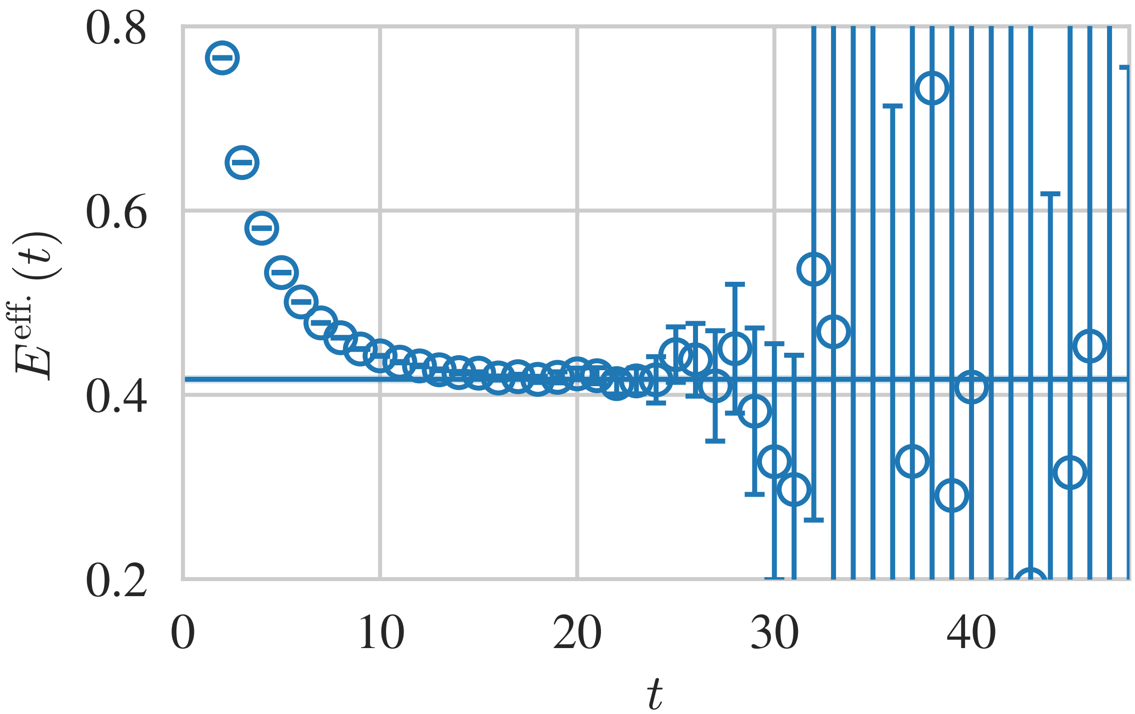

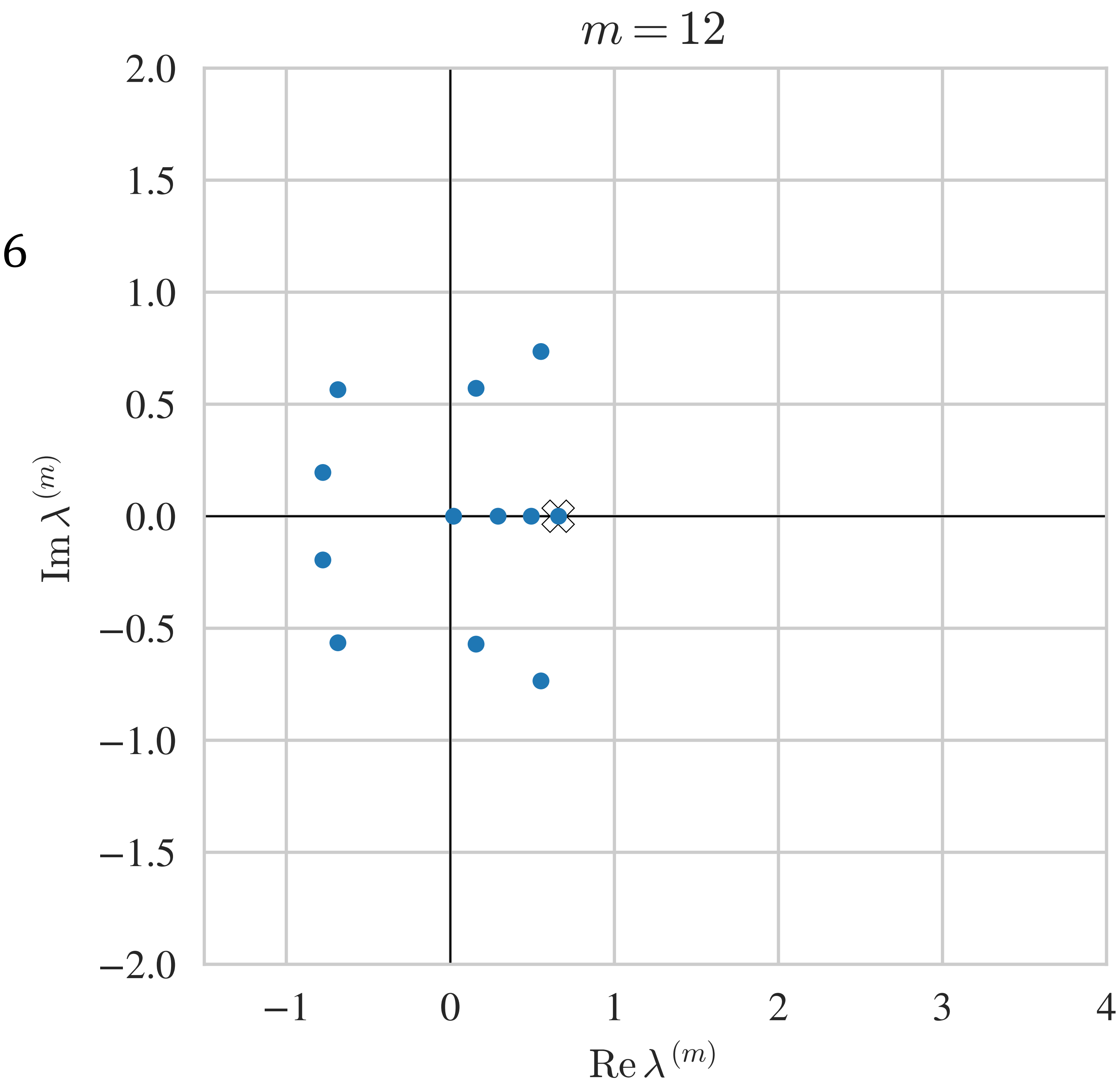

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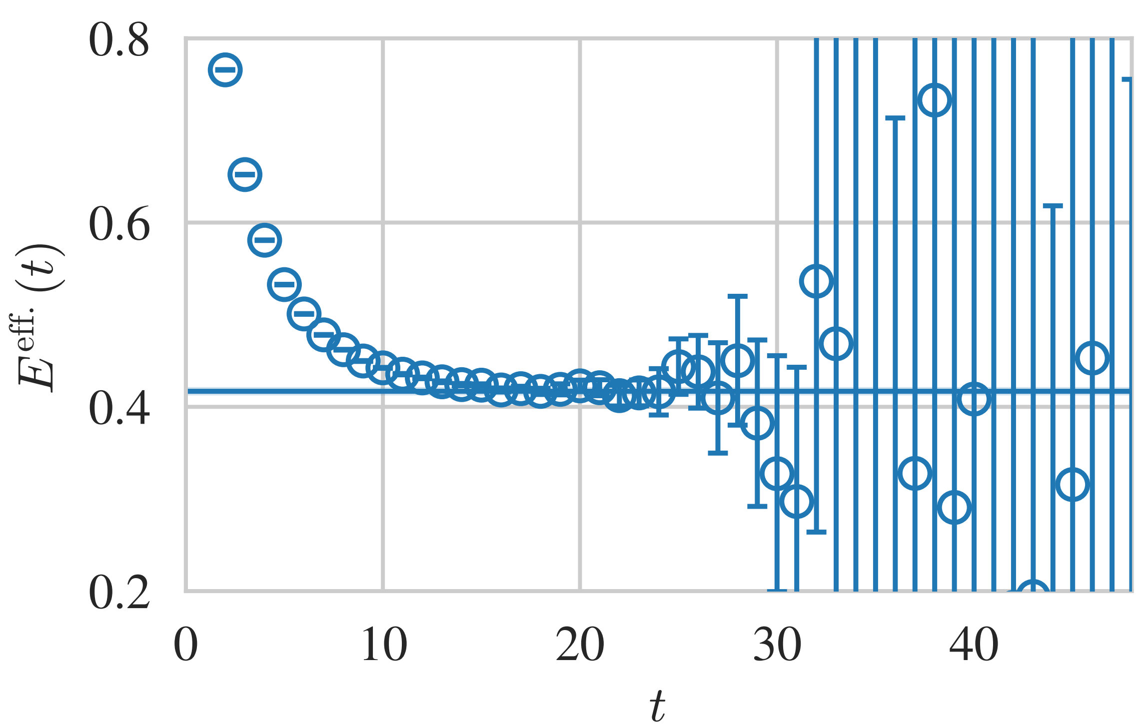

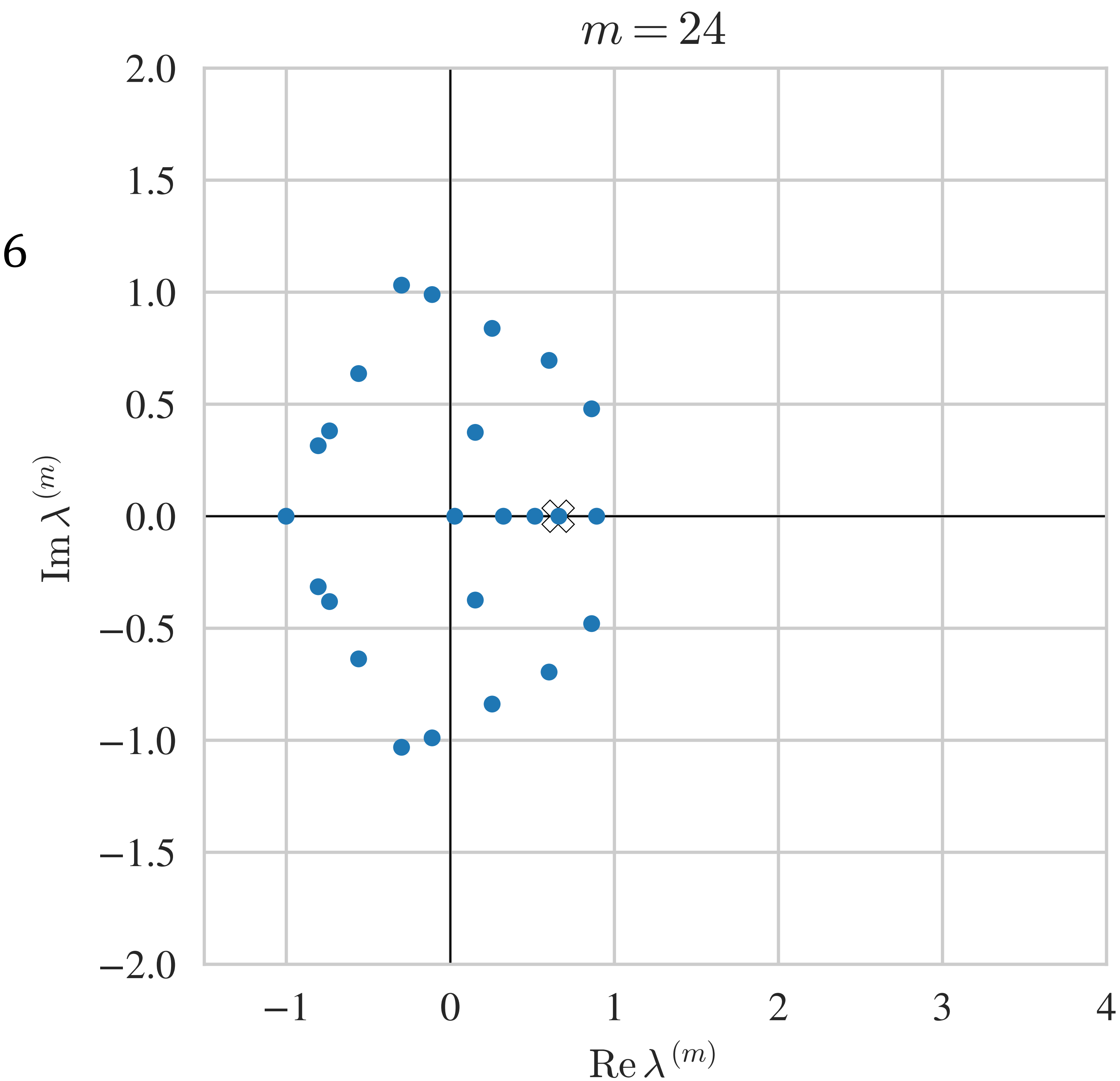

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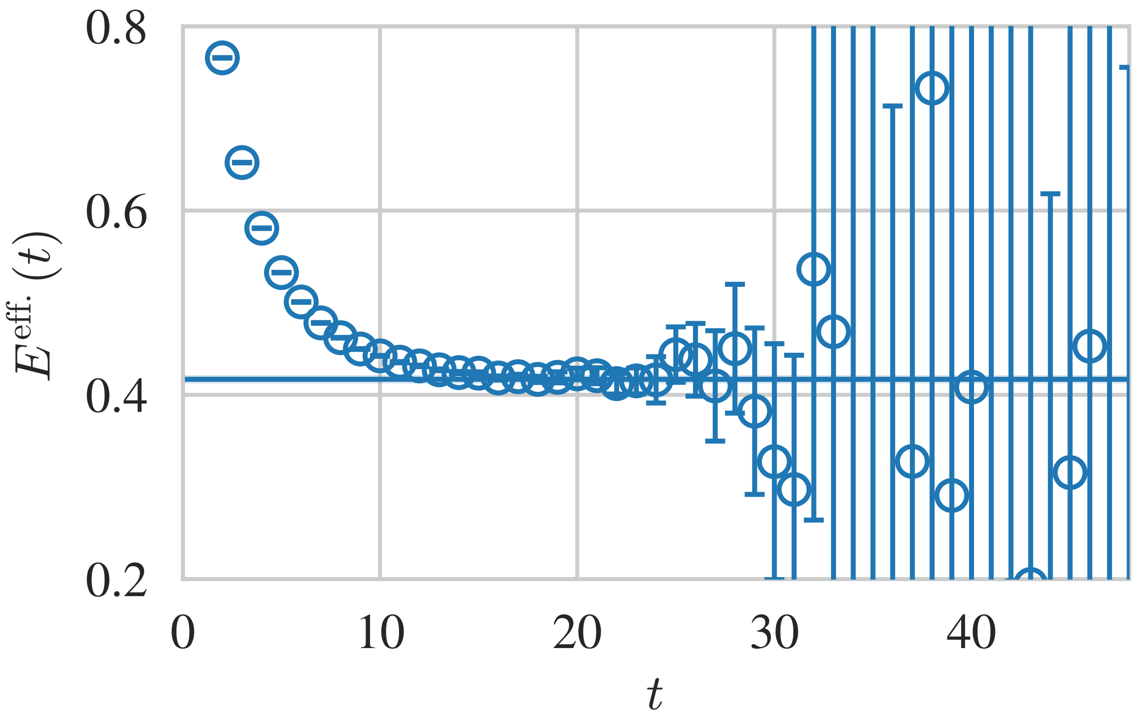
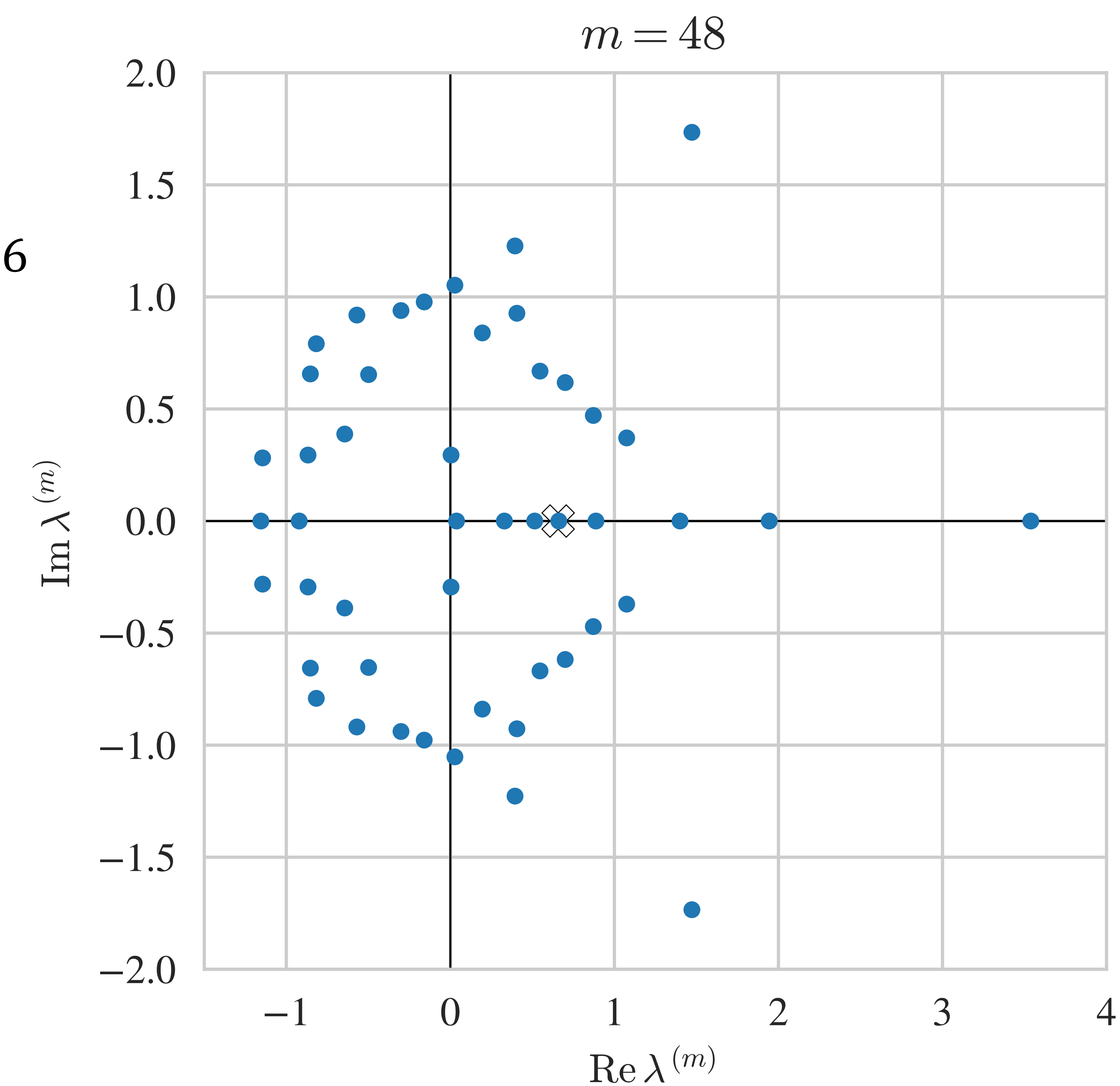
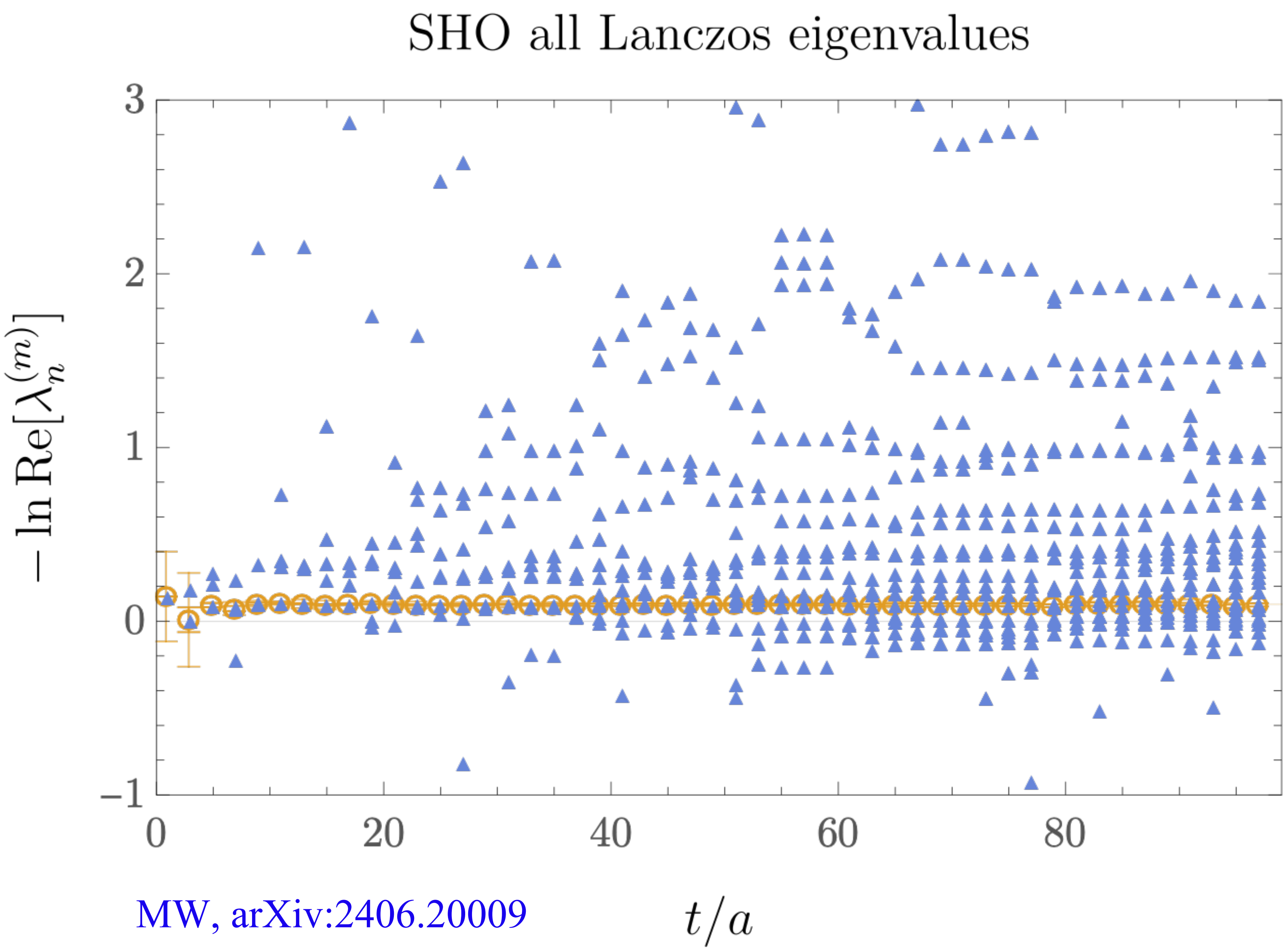




Is it really that easy?

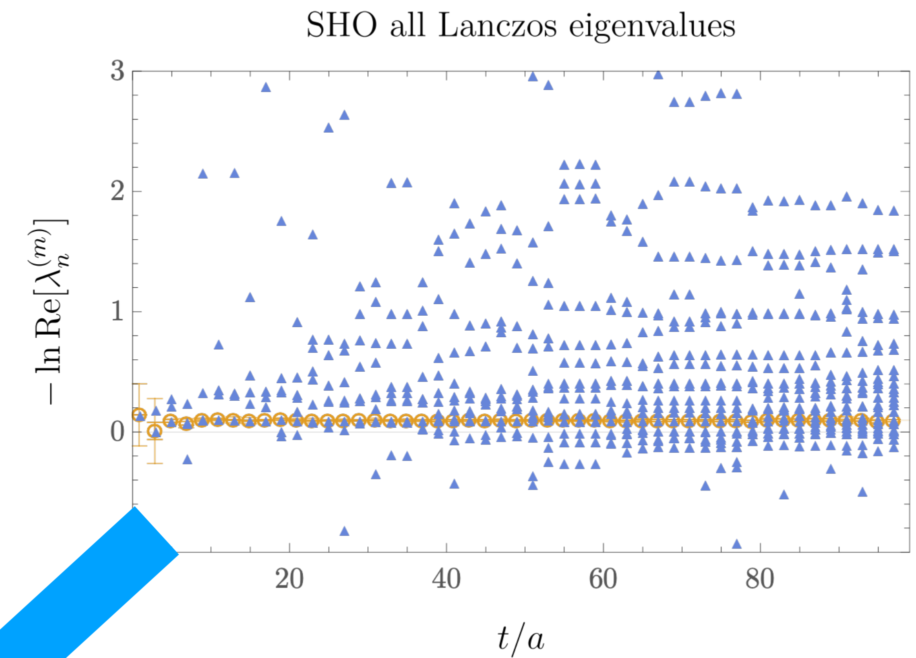
- No
- Lanczos produces an increasingly dense forest of “spurious eigenvalues”

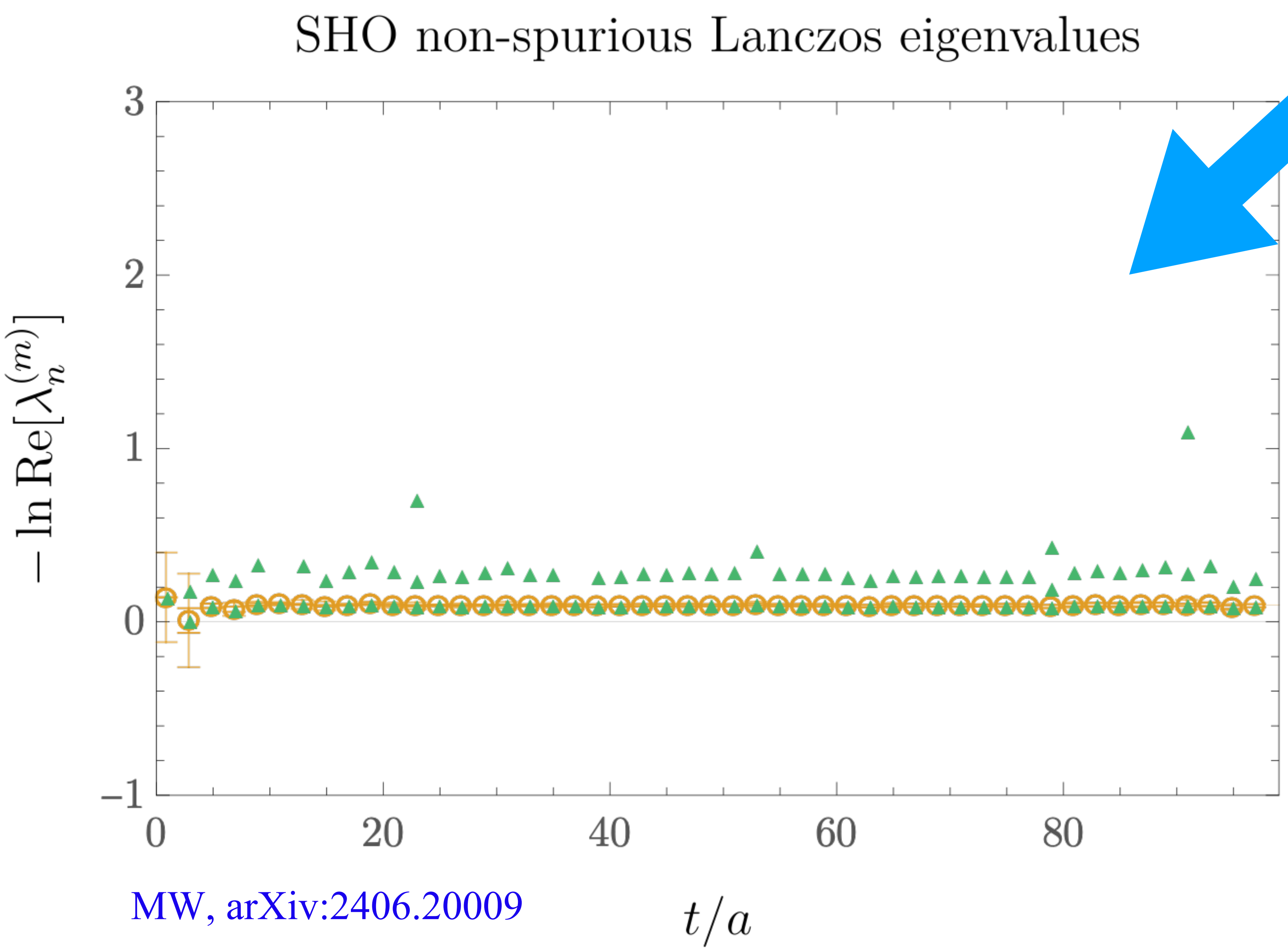


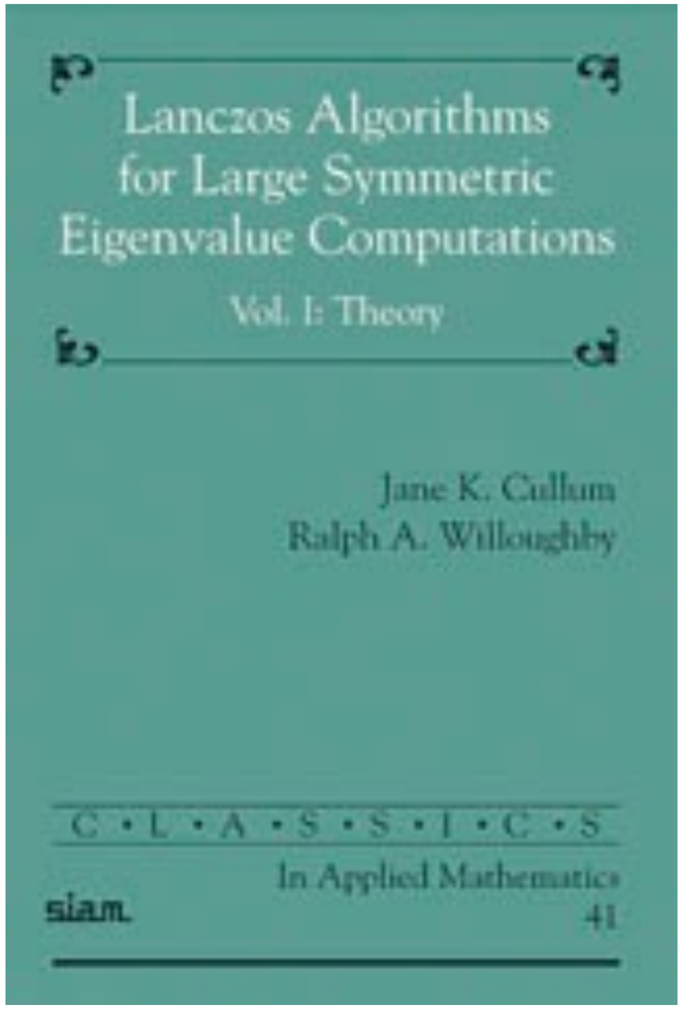
MW, arXiv:2406.20009

Spurious eigenvalues

- We need a way to automatically detect which eigenvalues are spurious and get rid of them







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Cullum-Willoughby

- Jane Cullum and Ralph Willoughby developed a useful criterion for identifying spurious eigenvalues in 1981

Cullum and Willoughby, Journal of Computational Physics 44, 329 (1981)

DEFINITION 1. Spurious ≡ Outwardly similar or corresponding to something without having its genuine qualities.

$$T^{(m)} = \begin{pmatrix} \alpha_1 & \beta_2 & & & & 0 \\ \gamma_2 & \alpha_2 & \beta_3 & & & \\ & \gamma_3 & \alpha_3 & \ddots & & \\ & & \ddots & \ddots & \beta_{m-1} & \\ & & & \gamma_{m-1} & \alpha_{m-1} & \beta_m \\ 0 & & & & \gamma_m & \alpha_m \end{pmatrix}$$

$$T_2^{(m)} = \begin{pmatrix} \times & \times & & & & 0 \\ \times & \alpha_2 & \beta_3 & & & \\ & \gamma_3 & \alpha_3 & \ddots & & \\ & & \ddots & \ddots & \beta_{m-1} & \\ & & & \gamma_{m-1} & \alpha_{m-1} & \beta_m \\ 0 & & & & \gamma_m & \alpha_m \end{pmatrix}$$

DEFINITION 2. Any simple eigenvalue of T_m that is pathologically close to an eigenvalue of $\hat{T}_2$ will be called "spurious."

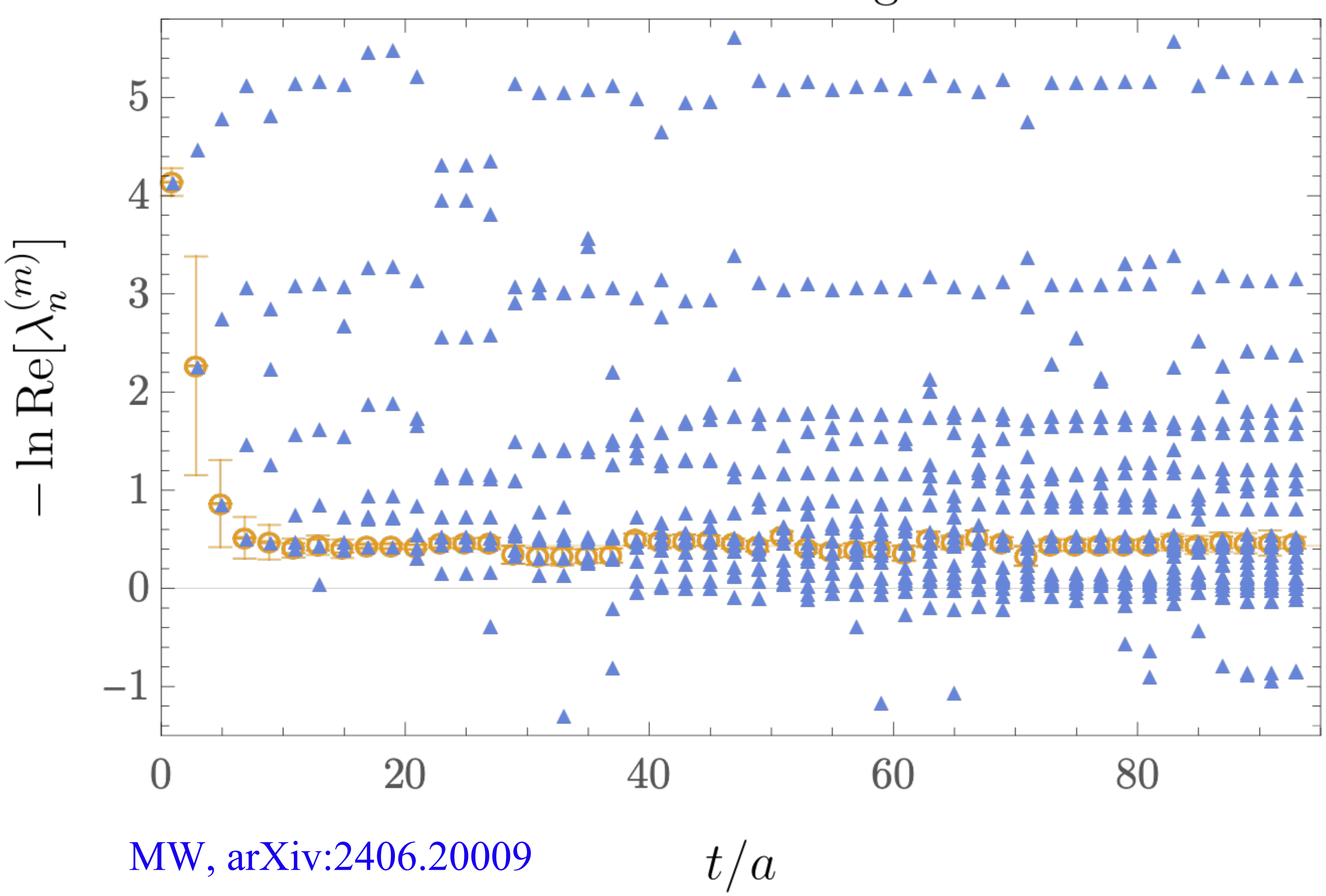
Think positive

- Since transfer matrix is positive-definite by assumption, any eigenvalues with non-zero imaginary parts can be discarded as spurious

- “Non-zero” can be kept exact even in the presence of noise by adopting oblique Lanczos formalism

  Saad, SIAM 19 (1982)

Proton all Lanczos eigenvalues



MW, arXiv:2406.20009

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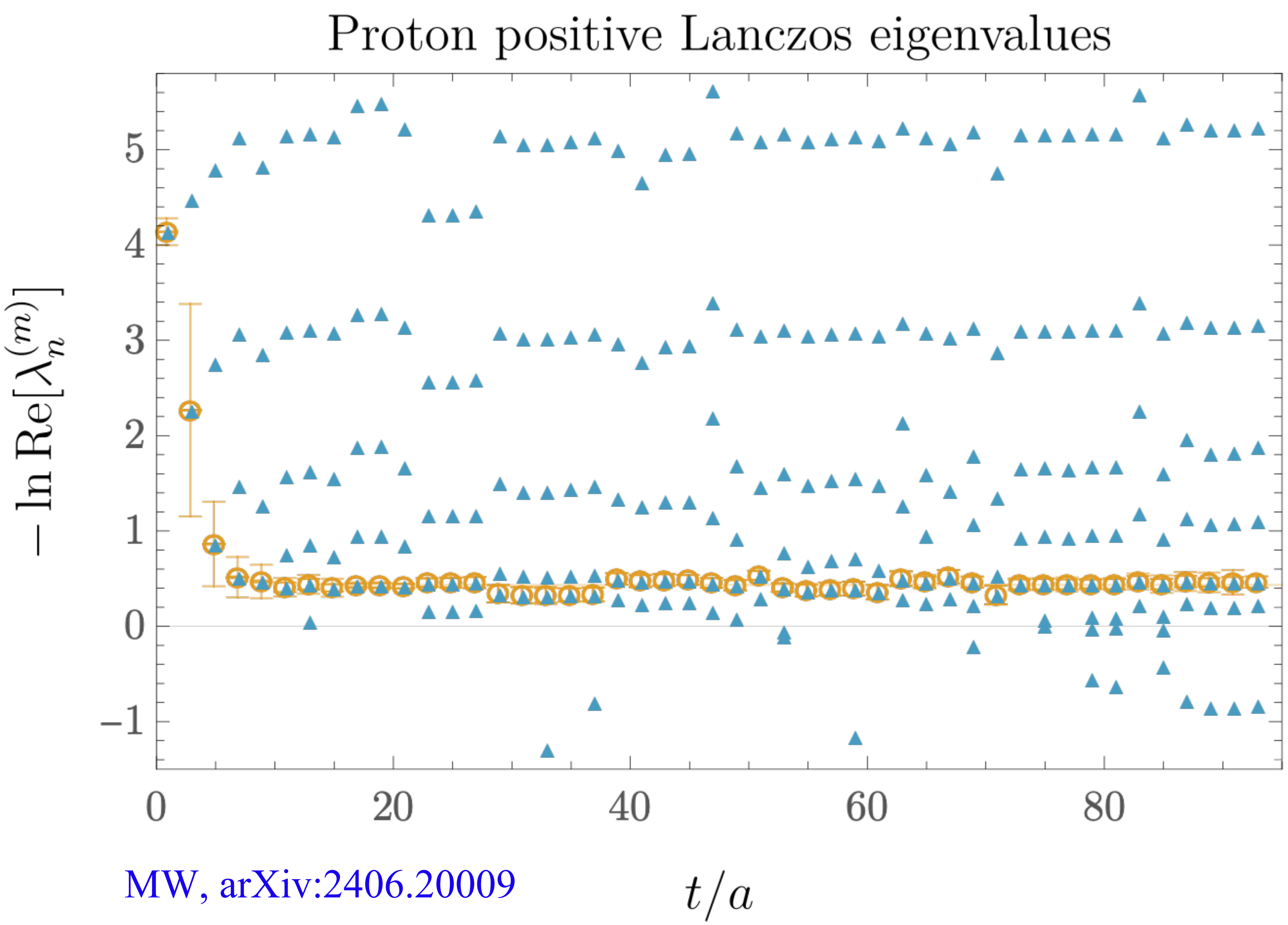


MW, arXiv:2406.20009

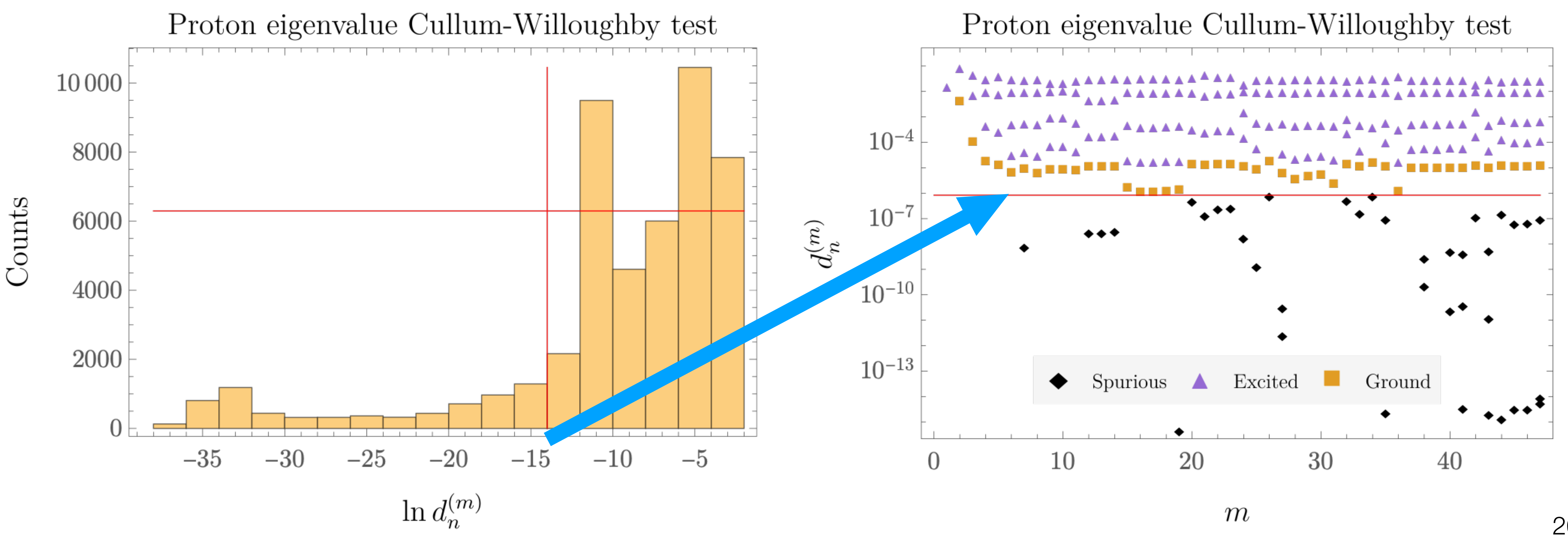
- This gets rid of many spurious eigenvalues but still leaves some that must be wrong because they correspond to $M_N < m_\pi$

Bootstrapping Cullum-Willoughby

- Defining "pathologically close" is easy for finite matrices with floating-point roundoff error, harder for Monte Carlo simulations of infinite-dimensional matrices

DEFINITION 1. Spurious ≡ Outwardly similar or corresponding to something without having its genuine qualities.

- Distances between $T^{(m)}$ and $T_2^{(m)}$ fluctuate due to noise much more for spurious than non-spurious eigenvalues
- Use bootstrap histograms to define cutoff

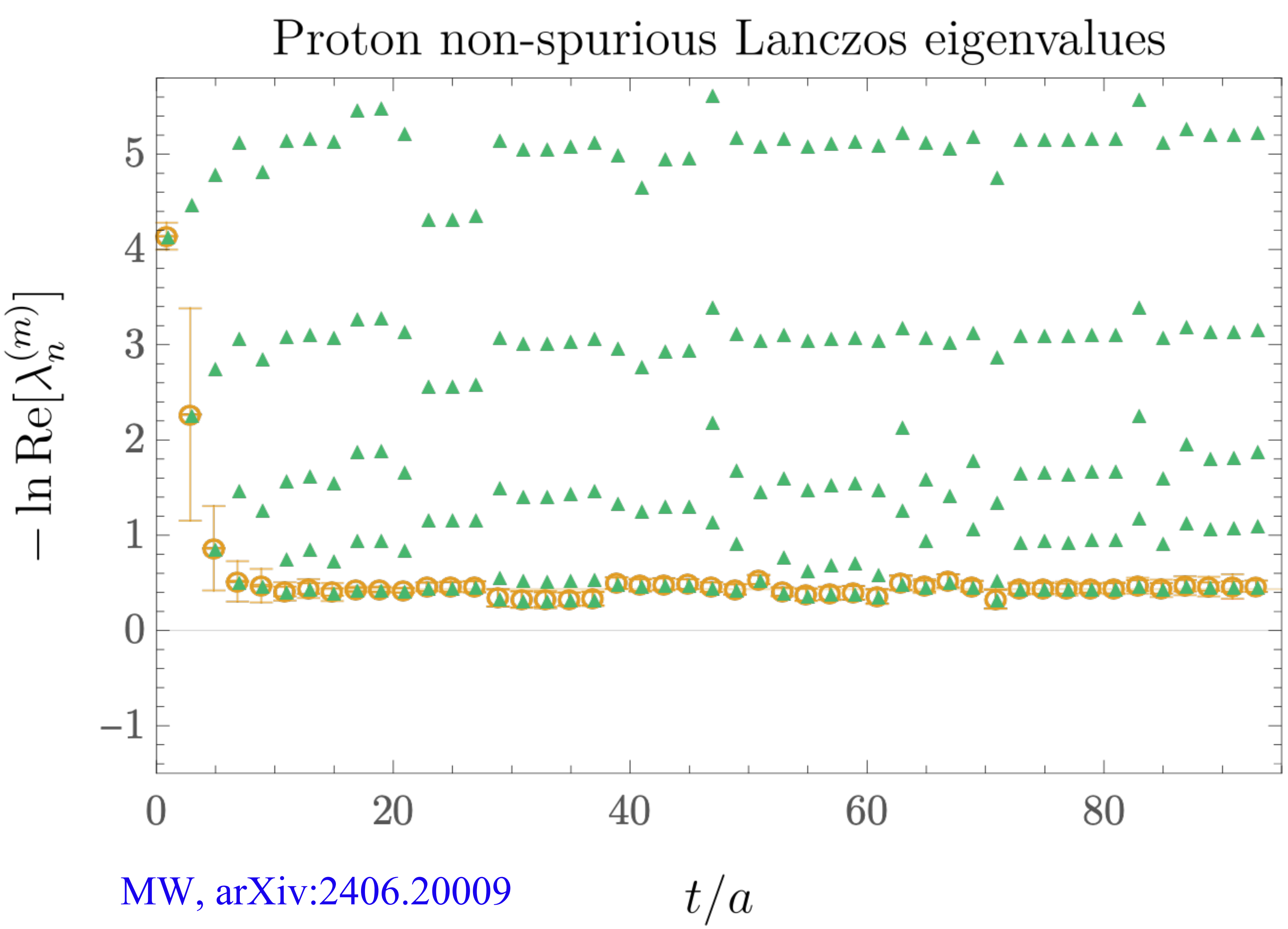


Non-spurious proton energies

- Largest eigenvalue not removed as spurious defines ground-state energy

$$E_0 = -\ln\lambda_0^{(m)}$$

- Excited-state energies also accessible



MW, arXiv:2406.20009

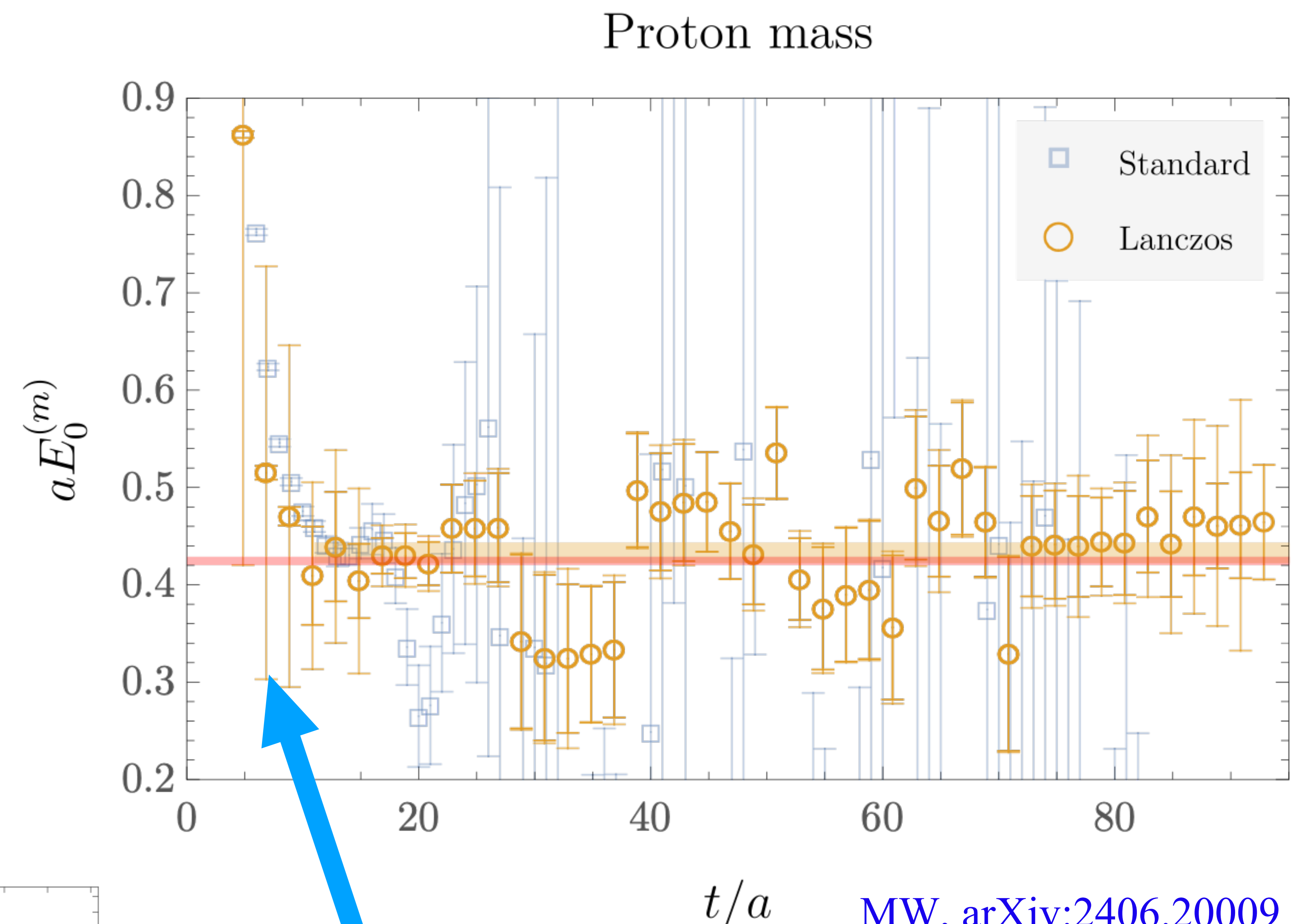
Outline

- Spectroscopy and the transfer matrix
- Lanczos spectroscopy algorithm
- “Spurious eigenvalues”
- **Proof-of-principle demonstrations**

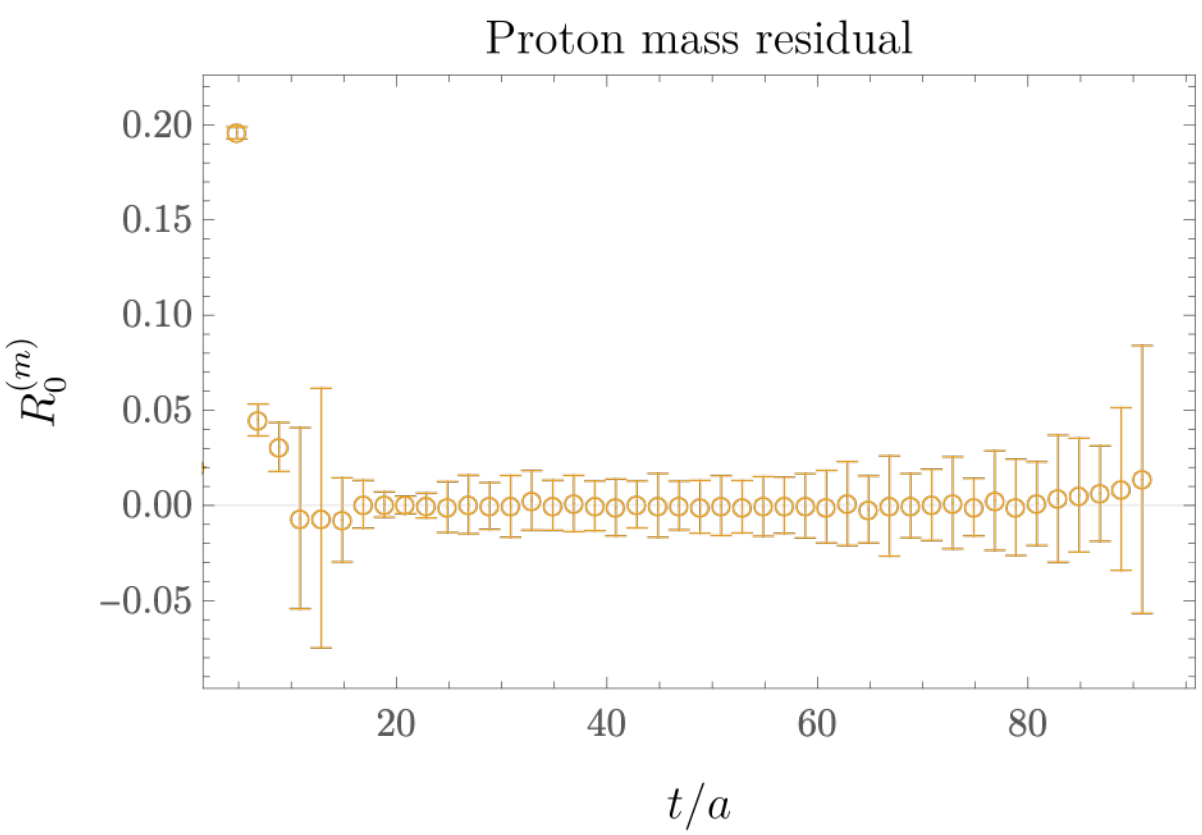
Lanczos proton mass results

- Bootstrap uncertainties complicated by outliers due to spurious eigenvalue misidentification within bootstrap samples

- Robust estimators e.g. based on confidence intervals critical



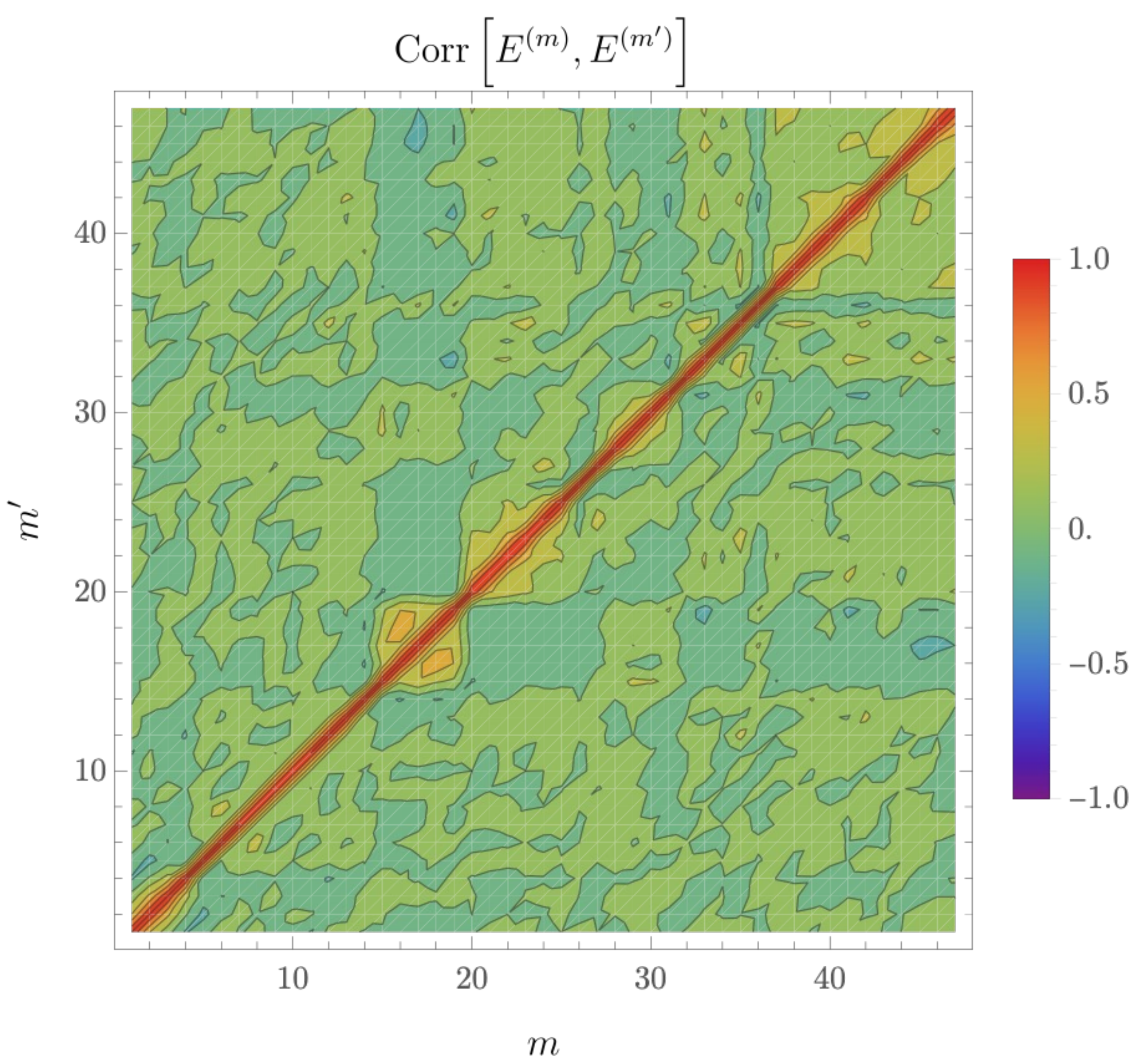
MW, arXiv:2406.20009

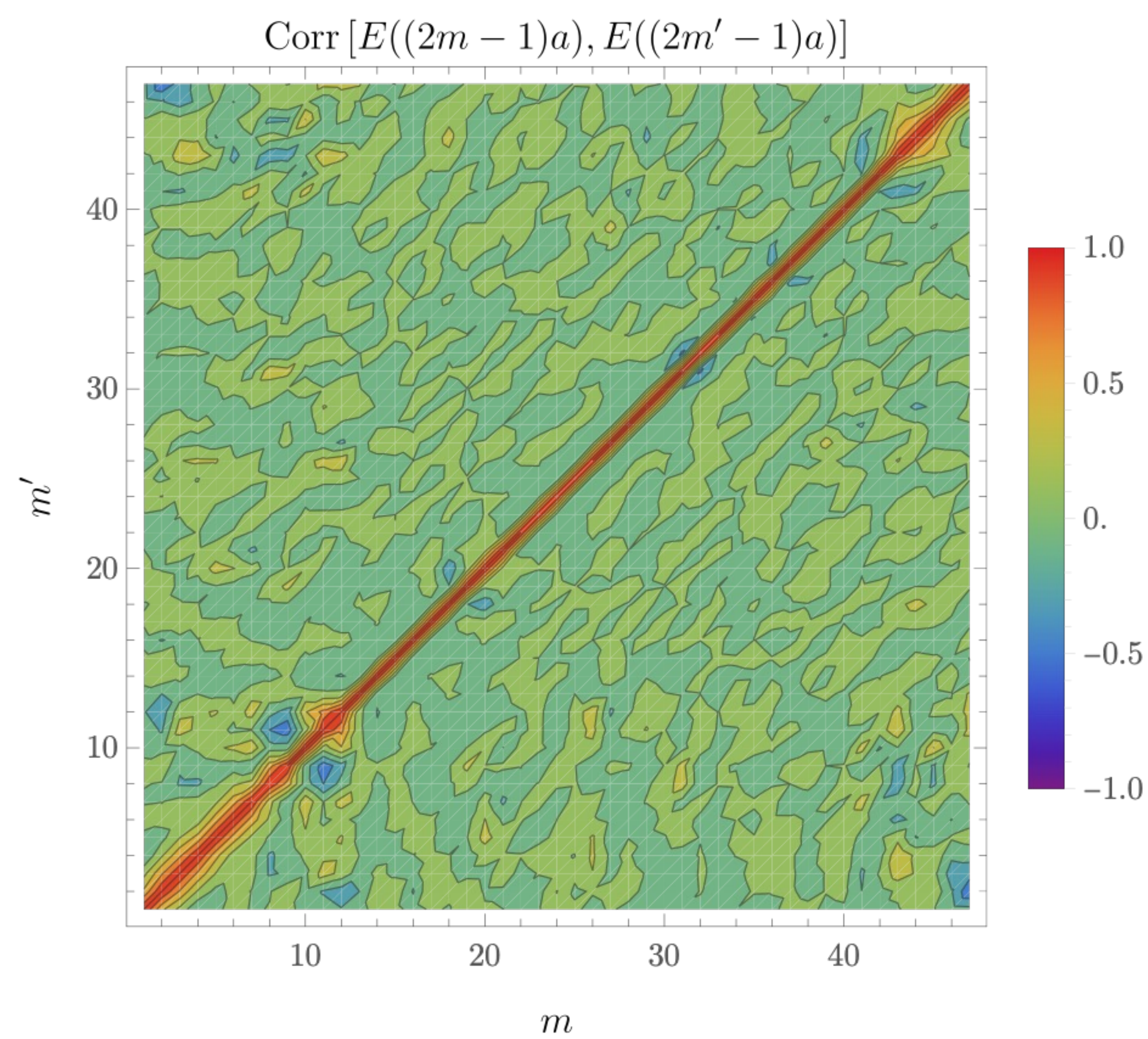


- Residual bound can be used to identify when Lanczos results have converged, provides bound on finite-t approximation errors

Correlations

- Correlations between Lanczos results at different imaginary times fall off rapidly with similar scale to correlations between standard effective mass results



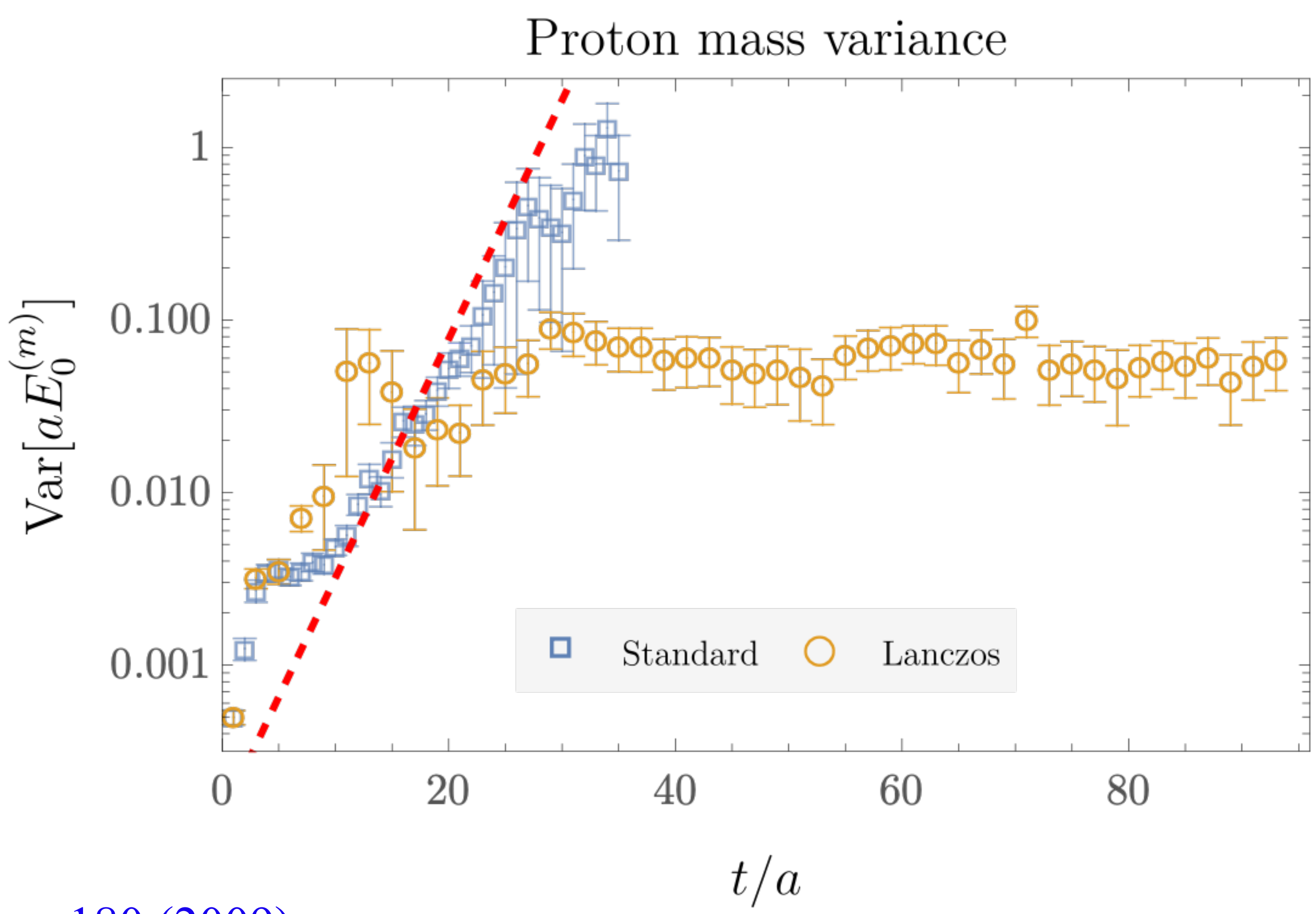


MW, arXiv:2406.20009

Projecting out the noise

- Signal-to-noise of Lanczos results does not degrade exponentially for large t

Why?



- Projection operator solution to signal-to-noise problem:

Della Morte and Giusti, Comp. Phys. Communications 180 (2009)

$$\langle \mathcal{O}(t)\overline{\mathcal{O}}(0)\rangle \longrightarrow \langle \mathcal{O}(t)P\overline{\mathcal{O}}(0)\rangle$$

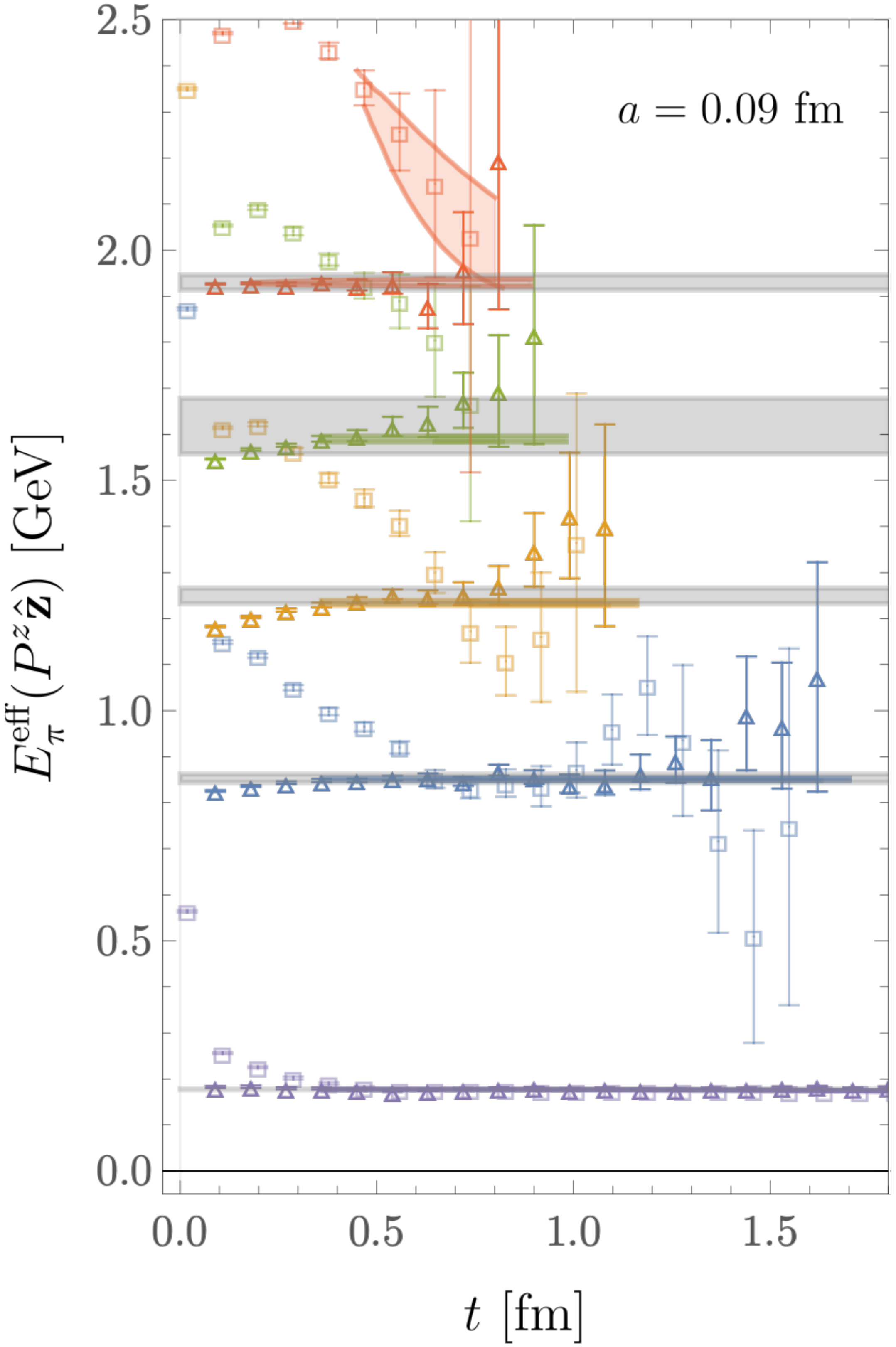
removes states from variance without quantum numbers of “signal squared,” e.g. three-pion states in nucleon variance

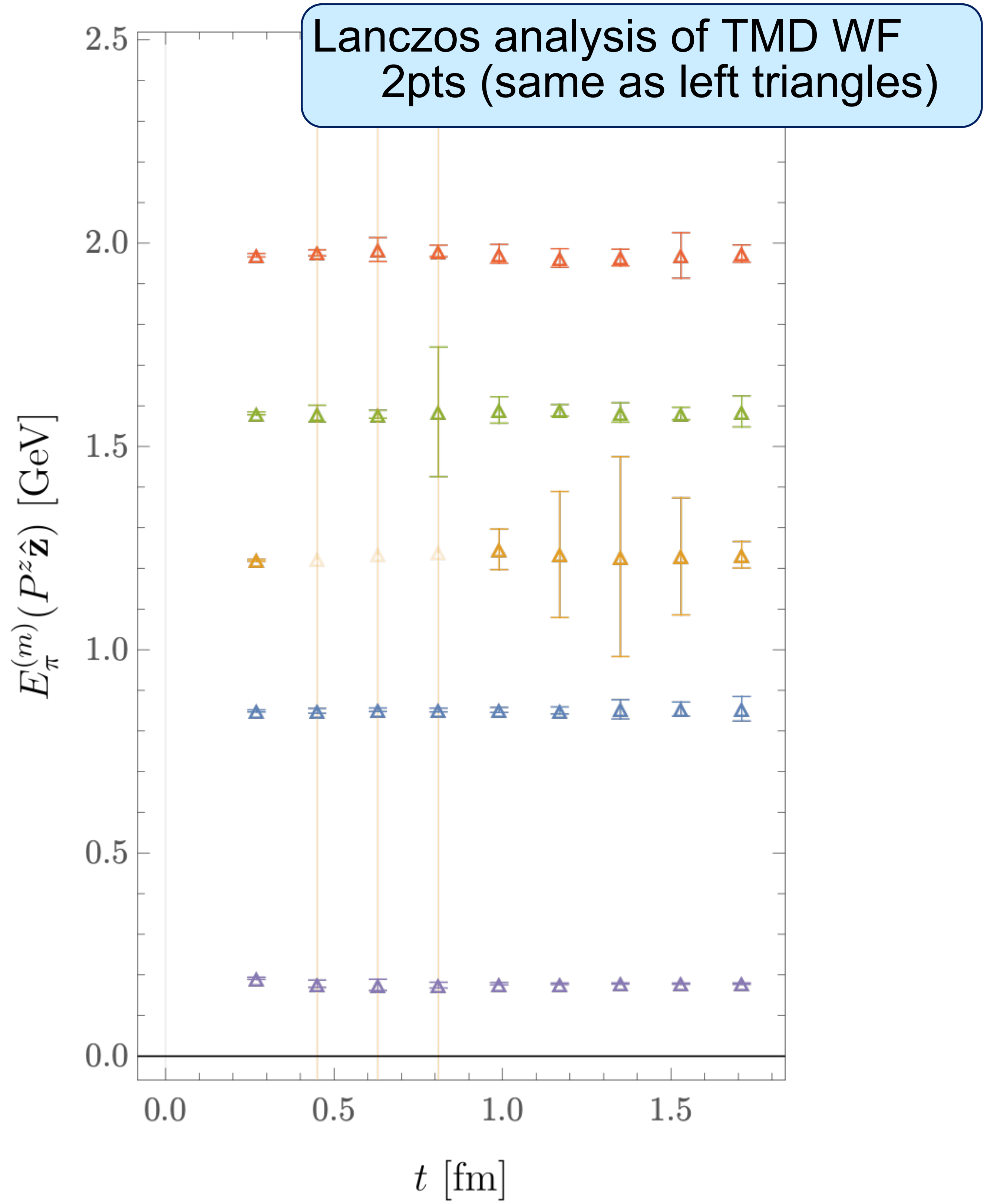
- Building such projectors is hard — but Lanczos provides Krylov-space approximations

$$P_n^{(m)} \equiv |y_n^{(m)}\rangle\langle y_n^{(m)}| \approx |n\rangle\langle n|$$

Saad, SIAM 17 (1980) Saad, SIAM 19 (1982)

Boosted states are noisy

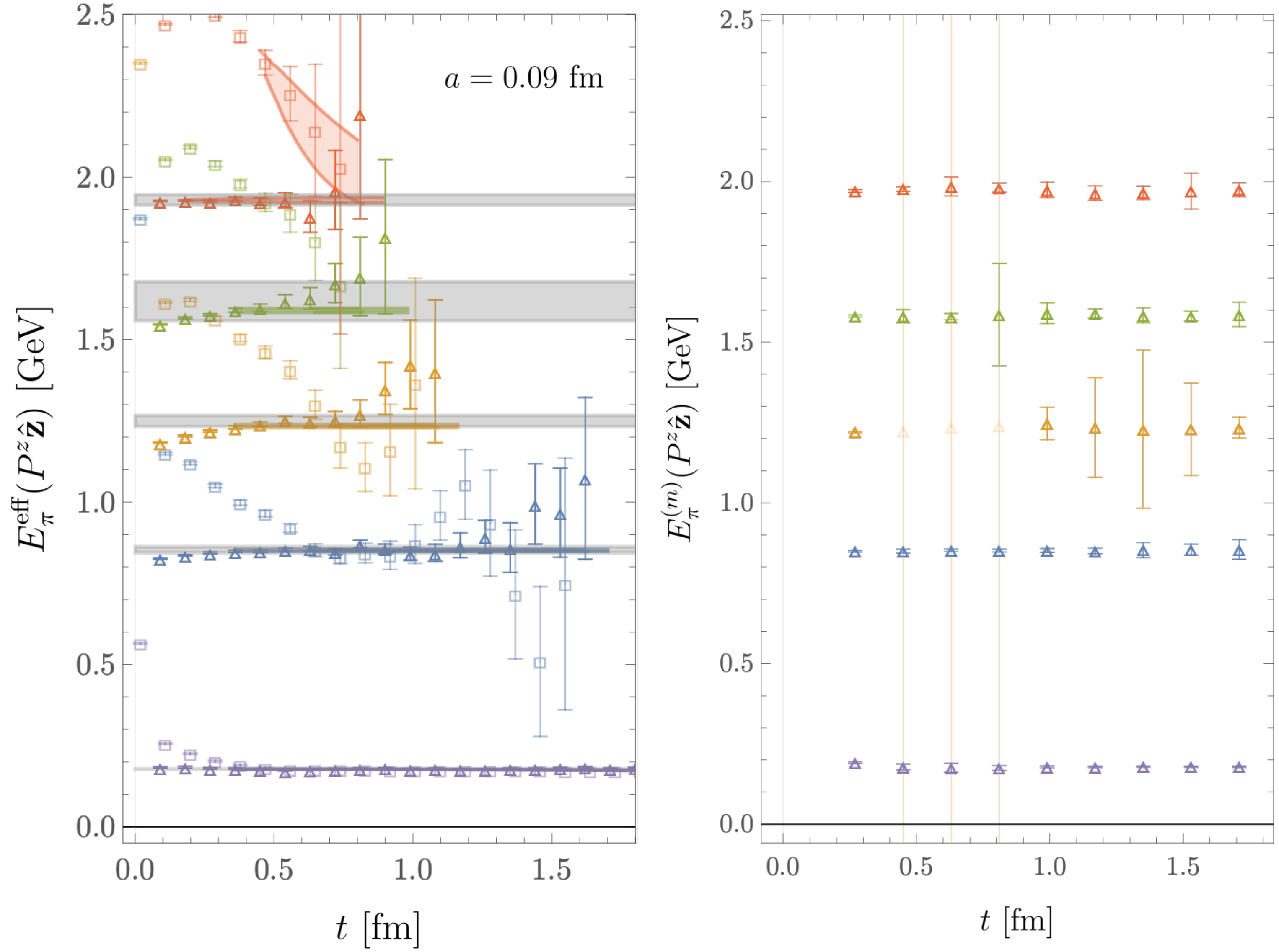


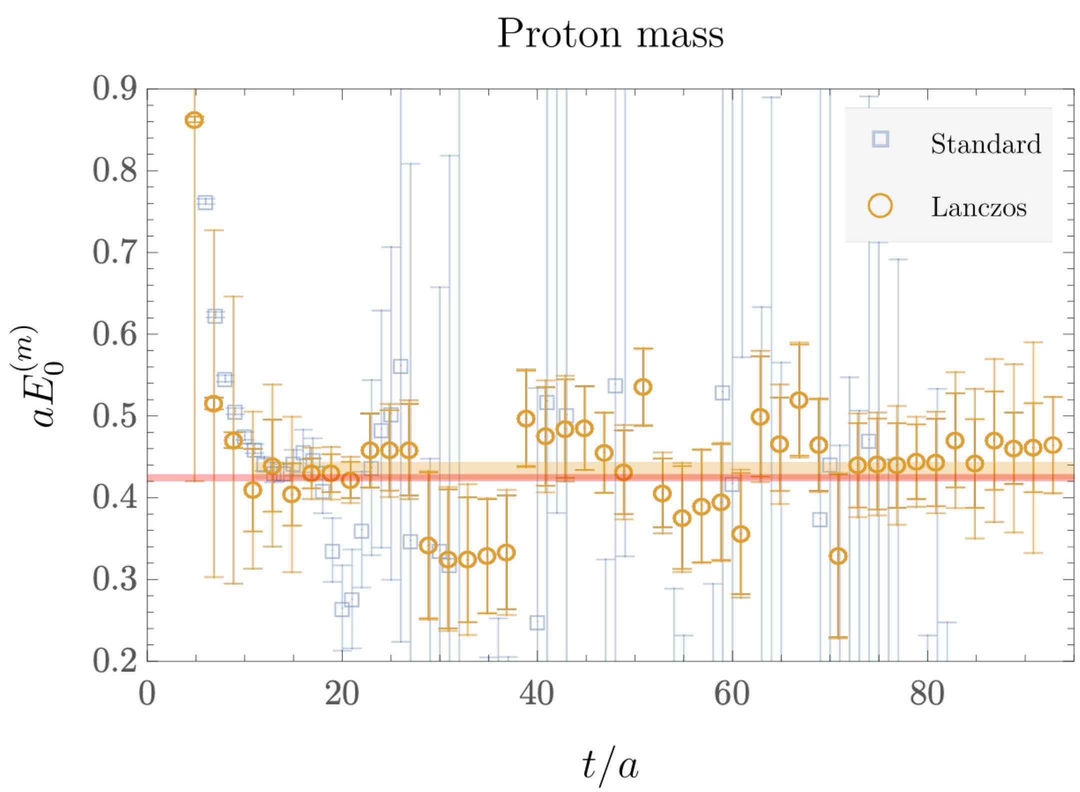


Avkhadiev, Shanahan, MW, Zhao, PRL 132 (2024)

Conclusions

- Lanczos enables rapid convergence even with small energy gaps
- Two-sided error bounds allow excited-state effects to be fully quantified
- Lanczos results do not show exponential signal-to-noise degradation





- Spurious eigenvalues lead to challenges: Cullum-Willoughby + bootstrap sufficient?

Qualitatively better properties than previous approaches to spectroscopy

…but what about matrix elements?