

Meson distillation profiles and their applications

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The Distillation Method

Replace $\psi \rightarrow VV^\dagger\psi$, where V contains the N_v lowest eigenmodes of the 3D Laplacian operator. [M. Peardon et al. (2009)]

Focus: Meson operator $\bar{\psi}\Gamma\psi$
($\Gamma = \gamma_5, \gamma_i, \nabla_i, \dots$) at 0 spatial momentum.

Building blocks

- Laplacian eigenvectors $V[t]$
- Perambulators
 $\tau[t_1, t_2] = V^\dagger[t_1]D^{-1}V[t_2]$
- Elementals $\Phi[t] = V^\dagger[t]\Gamma V[t]$

Advantages

- ✓ Perambulators/elementals have manageable sizes.
- ✓ Perambulators are independent from elementals.

Disadvantages

- ✗ N_v scales with 3D physical lattice volume.
- ✗ Many inversions required.

Developing an improvement

How to choose N_v ? **Physical** and **numerical** issues.

Too small:

- **Neglects** significant low energy modes. **Over-smearing!**

Too large:

- **Expensive.** **Number of eigenvectors, inversions and size of matrices.**
- Can include **non-significant** modes. **Under-smearing!**

Is a given N_v equally good for all states? **One-for-all might not be the best choice.**

- Different Γ correspond to different J^{PC} with **different** spatial properties.
- **Excited states** of a same J^{PC} can also further differ.

Let's begin with some N_v and see what we can learn...

Step 1: Calculate $V[t]$

Solve the sparse H.P.D eigenproblem $-\nabla^2[t]v_i[t] = \lambda_i[t]v_i[t]$ via the Lanczos algorithm with some improvements:

- ✓ Chebyshev acceleration $\rightarrow P(-\nabla^2[t])v_i[t] = P(\lambda_i[t])v_i[t]$. Improved convergence with spread-out spectrum. [D. C. Sorensen and C. Yang (1997)]
- ✓ Periodic reorthogonalization. Cheaply monitor orthogonality and fix only when necessary. [J. F. Grcar (1981)]
- ✓ Thick-Restart scheme. Limit memory requirements. [K. Wu and H. Simon (2000)]
- ✓ MR³ eigensolver for tridiagonal eigenproblem in LAPACK. $\mathcal{O}(m^2)$ for eigenpairs. [I. S. Dhillon and B. N. Parlett (2004)]
- ✓ Time parallelization. Different values of t can be analyzed simultaneously.

Further modifications are possible: Refined vectors [Z. Jia (1997)], ...

Step 2: Calculate $\Phi[t]$

Numerical considerations:

- Γ in Dirac space $\rightarrow \Phi[t]_{\alpha\beta}^{ij} = \delta_{ij}\Gamma_{\alpha\beta}$. No extra cost and useful sparsity.
- $\Gamma = \mathcal{H}\mathcal{D}$ in Space/Color/Dirac $\rightarrow \Phi[t]_{\alpha\beta}^{ij} = v_i[t]^\dagger \mathcal{D}[t] v_j[t] \mathcal{H}_{\alpha\beta}$. No sparsity but symmetry can reduce the number of operations required.
- Parallelization in time. Same advantage as in Lanczos.

A physical consideration: Can we use the vectors in a better way?

\rightarrow **Starting point:** Quark distillation profile $g(\lambda)$ used via $\psi \rightarrow VJV^\dagger\psi$ with $J[t]_{ij} = \delta_{ij}g(\lambda_i[t])$. Modulate contribution from each vector.

The **major** improvement comes in this step.

Step 3: Calculate $\tau[t_1, t_2]$

Numerical considerations:

- Solve systems $Dx^{(i,\alpha,t)} = v_{i,\alpha}[t]$. Use your preferred solver.
- $v_{j,\beta}[t']^\dagger x^{(i,\alpha,t)}$ can be done cheaply. Unnecessary operations are avoided.
- These inner products can also be parallelized in time.
- ! Some considerations might lead to improvements of the solver. [More details at the end.](#)

Towards an improved elemental

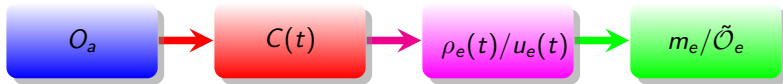
Our case: Fix Γ and study ground/excited states via a GEVP formulation.

[C. Michael & I. Teasdale (1983)] [M. Lüscher & U. Wolff (1990)] [B. Blossier et al. (2009)]

- Variational basis: $\mathcal{O}_a = \bar{\psi}_a \Gamma \psi_a$ with $\psi_a = V J_a V^\dagger \psi$.
- Correlation matrix $C_{ab}(t) = \langle \mathcal{O}_a(t) \bar{\mathcal{O}}_b(0) \rangle$
 - Pruning via SVD recommended for numerical stability.

[J. Balog et al. (1999)], [F. Niedermayer et al. (2001)]

- Solve GEVP $C(t)u_e(t, t_0) = \rho_e(t, t_0)C(t_0)u_e(t, t_0)$.
 - Eigenvalues $\rho_e(t, t_0)$ give access to masses of the different states.
 - Eigenvectors $u_e(t, t_0)$ allow to build an operator $\tilde{\mathcal{O}}_e$ with the largest overlap with the wanted energy eigenstate from the basis elements.



Optimal meson distillation profiles

The **new** improvement: For a fixed Γ and energy level e one can build an optimal elemental given by

$$\tilde{\Phi}^{(\Gamma,e)}[t]_{ij} = \tilde{f}^{(\Gamma,e)}(\lambda_i[t], \lambda_j[t]) v_i[t]^\dagger \Gamma_{\alpha\beta} v_j[t]$$

which includes the **optimal meson distillation profile** given as

$$\tilde{f}^{(\Gamma,e)}(\lambda_i[t], \lambda_j[t]) = \sum_k \eta_k^{(\Gamma,e)} g_k(\lambda_i[t])^* g_k(\lambda_j[t]).$$

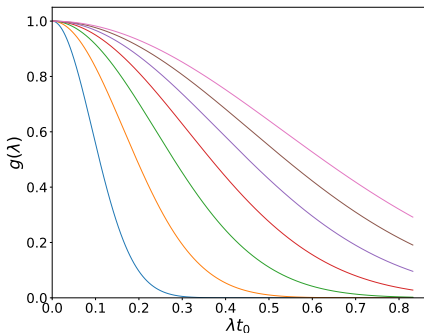
[F. Knechtli, T. Korzec, M. Peardon, J. A. Urrea-Niño, Phys. Rev. D106 (2022)]

Advantages:

- ✓ $C(t)$ requires **very little** additional cost to build. **Elementals required** come "for free" from the standard one.
- ✓ $\tilde{f}^{(\Gamma,e)}(\lambda_i[t], \lambda_j[t])$ tells us if N_v is large enough and how to use the N_v eigenvectors **for each Γ and energy state**. **An answer to our physical questions.**

Applying the method

- QCD with $N_f = 2$ at half the physical charm quark mass.
No light quarks. Clover-improved Wilson fermions.
- 48×24^3 and 96×48^3 lattices with $a \approx 0.0658, 0.049$ fm. Check effectiveness at smaller resolutions and larger volume.
- Both local and derivative Γ . [J. J. Dudek et al. (2008)]



- $g_i(\lambda) = e^{-\frac{\lambda^2}{2\sigma_i^2}}$ in this work.
Suppression of large λ follows distillation intuition.
- $g_i(\lambda) = \lambda^i$ was tried too.
Same result but less numerical stability. Avoided basis bias.

Objects of interest

Meson 2-point functions:

- $C_{ab}^V(t) = - \left\langle \text{Tr} \left(\Phi_a[t] \tau[t, 0] \bar{\Phi}_b[0] \tau[0, t] \right) \right\rangle$
- $C_{ab}^S(t) = C_{ab}^V(t) + \left\langle 2 \text{Tr} \left(\Phi_a[t] \tau[t, t] \right) \text{Tr} \left(\bar{\Phi}_b[0] \tau[0, 0] \right) \right\rangle$. Measured exactly.

Glueball-meson 2-point function:

- $C_{MG}(t) = \left\langle \text{Tr} \left(\Phi_a[t] \tau[t, t] \right) G[0] \right\rangle$

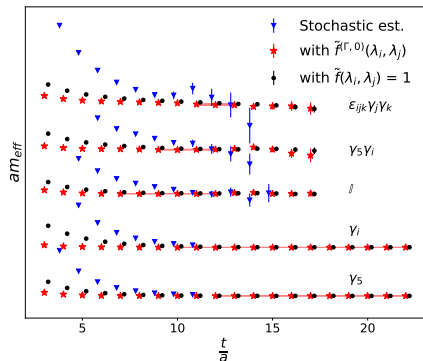
Effective masses (Simplified):

$$C_{ab}(t) = \sum_k \langle 0 | \hat{\mathcal{O}}_a | k \rangle \langle k | \hat{\mathcal{O}}_b^\dagger | 0 \rangle e^{-m_k t} \approx \langle 0 | \hat{\mathcal{O}}_a | g \rangle \langle g | \hat{\mathcal{O}}_b^\dagger | 0 \rangle e^{-m_g t}$$
$$\rho_e(t) \propto e^{-m_e t}$$

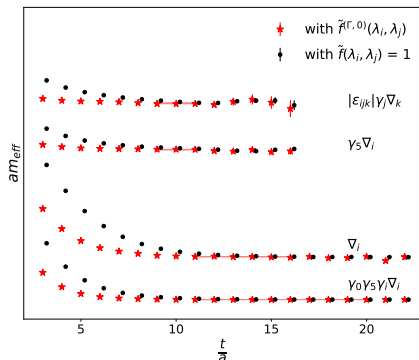
Goal of the method: Increase overlap with wanted state and decrease overlaps with unwanted states **without** much additional cost.

Coarse lattice ($L \approx 1.51 \text{ fm}$) with $N_v = 200$

Local iso-vector operators



Derivative iso-vector operators



Fractional overlaps:

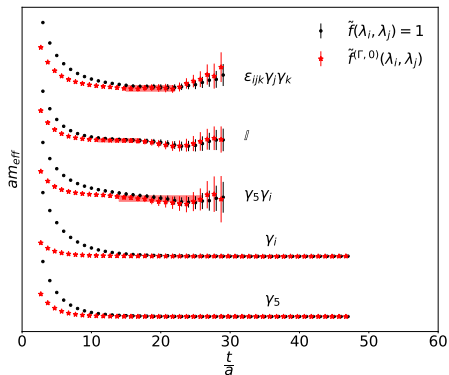
- γ_5 : $0.9272(3) \rightarrow 0.9858(2)$
- γ_i : $0.8743(10) \rightarrow 0.9900(5)$
- $\epsilon_{ijk}\gamma_j\gamma_k$: $0.77(7) \rightarrow 0.93(1)$

Fractional overlaps:

- ∇_i : $0.4758(7) \rightarrow 0.742(2)$
- $\gamma_5\nabla_i$: $0.84(1) \rightarrow 0.970(5)$
- $\mathbb{Q}_{ijk}\gamma_j\nabla_k$: $0.858(8) \rightarrow 0.981(3)$

Fine lattice ($L \approx 2.30 \text{ fm}$) with $N_v = 325$

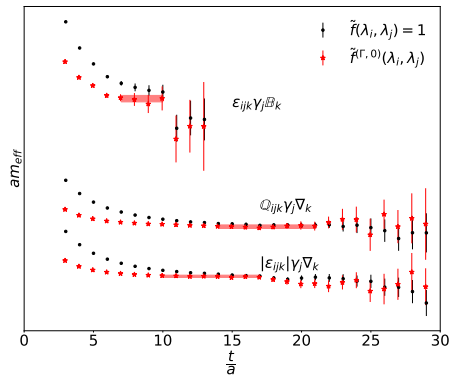
Local iso-vector operators



Fractional overlaps:

- γ_5 : $0.8765(7) \rightarrow 0.9555(5)$
- γ_i : $0.825(3) \rightarrow 0.969(2)$

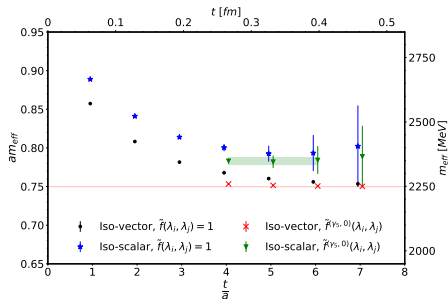
Derivative iso-vector operators



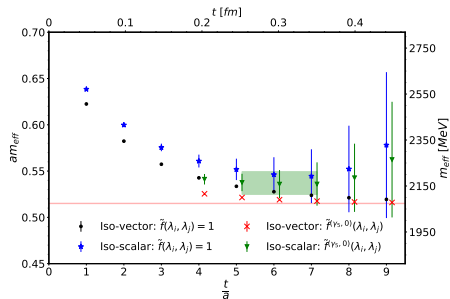
Fractional overlaps:

- $\mathbb{Q}_{ijk}\gamma_j\nabla_k$: $0.82(2) \rightarrow 0.92(1)$
- $\epsilon_{ijk}\gamma_j\mathbb{B}_k$: $- \rightarrow 0.91(1)$

Coarse lattice iso-scalar 0^{-+}

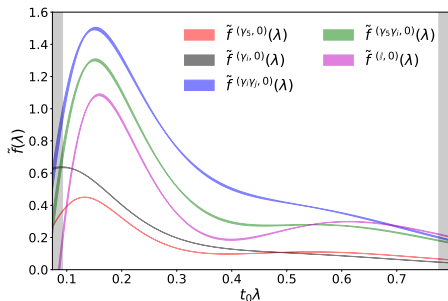


Fine lattice iso-scalar 0^{-+}

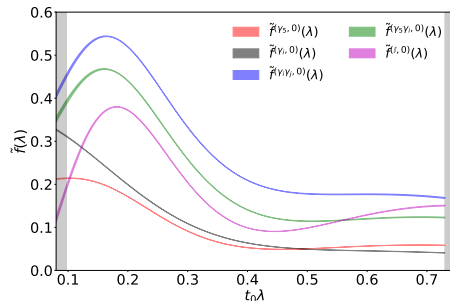


- Mass splitting is visible in both ensembles. Standard distillation already makes this possible.
- Optimal profile from iso-vector **improves** the iso-scalar too. Closeness in mass might mean similar profiles.

Optimal Profiles: Coarse lattice



Optimal Profiles: Fine lattice



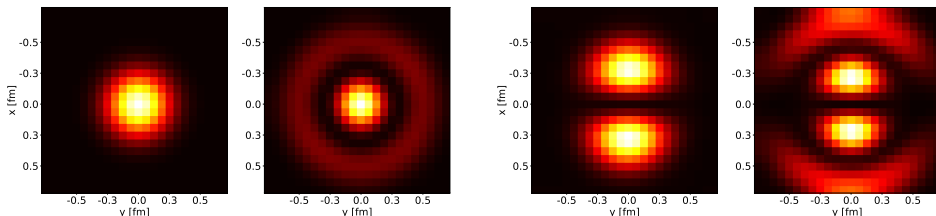
- $\tilde{f}^{(\Gamma,0)}(\lambda_i, \lambda_j) \neq 1$ always. Improvement over orthogonal projection.
- Suppression of large λ remains. Distillation intuition still holds.
- Different profile for different Γ . Profiles are unique.
- $\tilde{f}^{(\Gamma,0)}(\lambda_i, \lambda_j)$ at large λ_i, λ_j tells us if we have enough eigenvectors. More systematic criterion for choosing N_v .
- $N_v^{fine} = 325 \leftrightarrow N_v^{course} = 100$. Volume scaling is a good initial guide.

Spatial Profiles

Spatial profile can be recovered:

- $\Psi^{(\gamma_5, e)}(\vec{x}) = \frac{1}{N_t} \sum_t ||Tr \left(\gamma_5 V[t] \tilde{\Phi}^{(\gamma_5, e)}[t] V[t]^\dagger \right) \phi_0 ||^2$
- $\Psi^{(\gamma_5 \nabla_1, e)}(\vec{x}) = \frac{1}{N_t} \sum_t ||Tr \left(\gamma_5 V[t] \tilde{\Phi}^{(\gamma_5 \nabla_1, e)}[t] V[t]^\dagger \right) \phi_0 ||^2$

with ϕ_0 a 3D point source. Profiles dictate spatial structure.

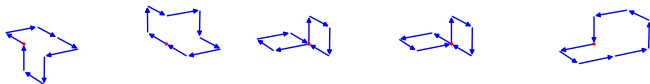


- Spatial behavior of state can be visualized.
- Finite-volume effects can be monitored.

Charmonium-Glueball mixing

To keep in mind:

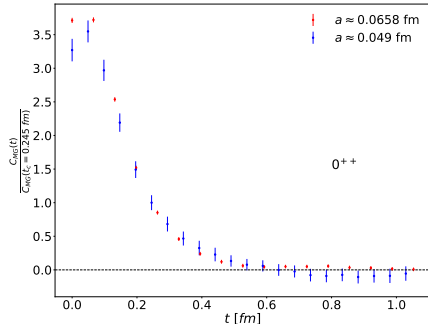
- Iso-scalar meson operators require disconnected pieces in correlation function. Feasible thanks to distillation.
- Glueballs are hard to find in un-quenched QCD. Optimal operators must be found via GEVP
 - 3D Wilson loops with different shapes and windings. [C. J. Morningstar & M. Peardon, (1999)] [B. Berg & A. Billoire, (1983)]



- Different smearing schemes and levels:
 - 3D-HYP [A. Hasenfratz & F. Knechtli, (2001)]
 - 3D improved APE [B. Lucini et al. (2004)]

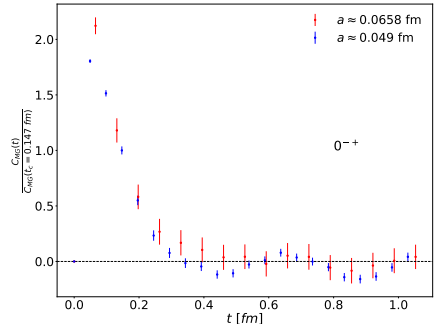
Scalar channel

$$0^{++} \rightarrow \Gamma = \mathbb{I}, \tilde{f}(\lambda_i, \lambda_j) = 1$$



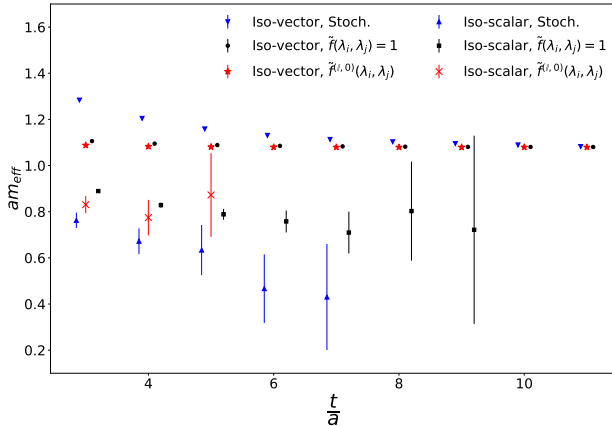
Pseudo-Scalar channel

$$0^{-+} \rightarrow \Gamma = \gamma_5, \tilde{f}^{(\gamma_5, 0)}(\lambda_i, \lambda_j)$$



- $C_{MG}(t) = \left\langle \text{Tr} \left(\Phi^{(\Gamma)}[t] \tau[t, t] \right) G^{(R^{PC})}(0) \right\rangle$.
- Correlators normalized at fixed time in physical units.
- Noise is dominated by the glueball. Blueballs require more statistics than mesons.

Why $\tilde{f}(\lambda_i, \lambda_j) = 1$ for 0^{++} ?



- There is a lighter iso-scalar state. Consistent with a scalar glueball.
- Significant mass difference \rightarrow Profiles might also be very different.
Unlike the 0^{-+} case.

About the perambulators...

We solve $Dx^{(i,\alpha,t)} = v_{i,\alpha}[t]$ for $x^{(i,\alpha,t)}$ **but** we only need $VV^\dagger x^{(i,\alpha,t)}$:

$$x^{(i,\alpha,t)} = \sum_{t_1=0}^{N_t-1} \sum_{\beta=0}^3 \sum_{j=1}^{N_v} \tau[t_1, t]_{\beta\alpha}^{ji} v_{j,\beta}[t_1] + \sum_{t_1=0}^{N_t-1} \sum_{\beta=0}^3 \sum_{j=N_v+1}^{3L^3} \tau[t_1, t]_{\beta\alpha}^{ji} v_{j,\beta}[t_1]$$

There are things we **know**, **want**, **don't know** and **don't want**.

→ We want a **very small** piece of the solution but we invest effort in finding **all** of it.

Additionally:

- RHS are sparse → V is block diagonal in time and spin.
- Solutions are $D^\dagger D$ -orthogonal.

Can we build a better solver taking all of these considerations into account?

Conclusions

Optimal meson distillation profiles can:

- ✓ **significantly** reduce excited state contamination at **no** extra inversion cost.
- ✓ serve as an **additional** degree of freedom for a GEVP formulation.
- ✓ reveal additional **spatial** information of the states of interest.
- ✓ be used for meson-glueball **mixing**.
- ✓ be applied to **hadron** operators and stochastic distillation.

and will be applied in an $N_f = 3 + 1$ ensemble with physical charm quark mass.

We improved the construction of the elementals. Can we do the same for the perambulators?

- We need only a **small** part of the solutions.
- The linear systems have some interesting properties.

Thank you for your attention!

Fractional overlap

Correlation function: Ground state + Excited state contamination

$$C(t) = 2c_0 e^{-m_0 \frac{T}{2}} \cosh \left(\left(\frac{T}{2} - t \right) m_0 \right) + B_1(t)$$

Normalized correlator:

$$C'(t) = \frac{C(t)}{C(t_0)} = \left(\frac{1 + B_2(t)}{1 + B_2(t_0)} \right) \frac{\cosh \left(\left(\frac{T}{2} - t \right) m_0 \right)}{\cosh \left(\left(\frac{T}{2} - t_0 \right) m_0 \right)}$$

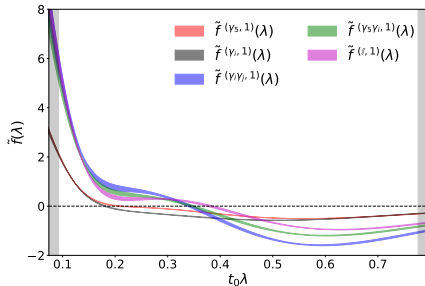
$$B_2(t) = \frac{B_1(t) e^{m_0 \frac{T}{2}}}{2c_0 \cosh \left(\left(\frac{T}{2} - t \right) m_0 \right)}$$

At mass plateau $B_1(t)$ is 0 and the fractional overlap can be fitted:

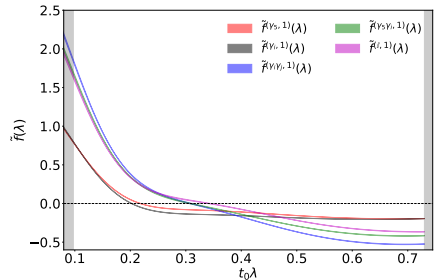
$$A_G = \frac{1}{1 + B_2(t_0)}$$

First excited state

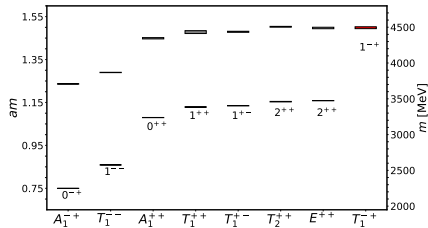
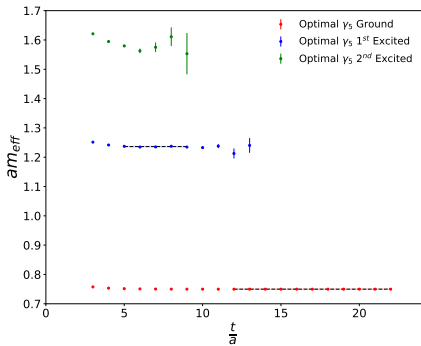
Optimal Profiles: Coarse lattice



Optimal Profiles: Fine lattice

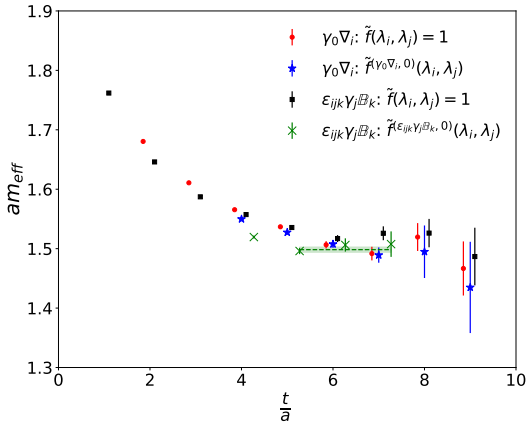


- A node appears for the first excited state.
- Same observations as for the ground state regarding the advantages of the different profiles.



- Inclusion of profiles grants access to excited states.
- Comparison to standard distillation requires using multiple Γ operators.

The spin-exotic 1^{-+}



- The $\epsilon_{ijk} \gamma_k \mathbb{B}_k$ operator **with** the optimal profile has the best overlap with the eigenstate.