Universität Münster

institut für theoretische physik

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NRW-FAIR Netzwerk

Lattice QCD applications of optimised meson operators in the distillation framework

HHIQCD 2024, Nishinomiya-Yukawa Workshop, YITP, Kyoto University

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Topics:

Lattice QCD

↪ Hadron Spectroscopy

↪ Distillation

↪ Profiles

↪ Applications

Who is involved:

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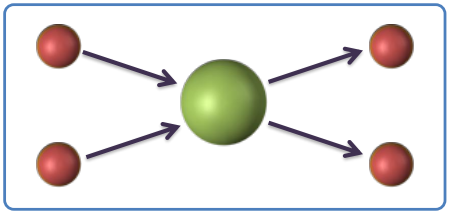
- *T. Korzec, U. Wuppertal*
- *J. Neuendorf, J. H., U. Münster*
- M. Peardon, Trinity College Dublin
- R. Höllwieser, *A. Risch, U. Wuppertal*
- L. Struckmeier, U. Wuppertal
- *J.A. Urrea-Niño, U. Wuppertal*

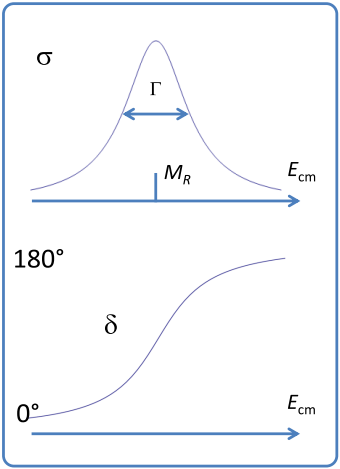
Outline:

1. Motivation & Basics
2. Distillation
3. Distillation profiles
4. Examples: Charmonium spectroscopy
5. Examples: D and D^* mesons
6. Profiles and momenta
7. Further applications
8. Summary & Outlook

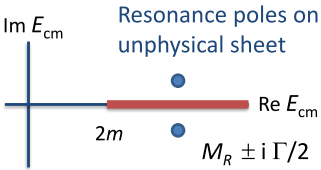
Scattering and resonances

Most hadrons = Resonances, decaying strongly to lighter hadrons





Singularity structure of scattering matrix (poles → state content)



Scattering and resonances

A scattering process such as **“two particles” → “two particles”** happens in real time

In **lattice QCD**, we work in Euclidean (imaginary) time

- Perfect for spectroscopy ↔ Systematically improvable, first-principles calculations
- However: *No* direct access to scattering
- Lüscher’s idea [M. Lüscher, NPB 354 (1991) 531] : Compute the two-particle spectrum in a *finite volume* and solve an equation to find the phase shifts and infer the resonance parameters
- Gives rise to a well-established workflow:

  Lattice QCD: Compute correlation matrix
  $\xrightarrow{\text{GEVP}}$ Obtain finite-volume spectrum
  $\xrightarrow{\text{Lüscher quant. cond.}}$ Determine scattering amplitudes
  $\longrightarrow$ Poles, couplings, ...

Scattering and resonances

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- Perfect for spectroscopy ↔ Systematically improvable, first-principles calculations
- However: *No* direct access to scattering
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- Practical "window" challenge: (1.) Effective masses $am_{\text{eff}} = \ln\left[C_{ij}(t)/C_{ij}(t+a)\right]$ approach ground state energy E_0 only at *large* t; (2.) Exponential *increase* of statistical errors at *large* t

⇒ Need operators with large overlaps onto eigenstates to get early plateaus already at *small* t (large variational basis, smearing); similar issue affects quark-line disconnected diagrams

→ We use quark smearing called **distillation** [M. Peardon et al., PRD 80 (2009) 054506]
with **profiles** [F. Knechtli, T. Korzec, M. Peardon, J.A. Urrea-Niño, PRD 106 (2022) 034501]

Spectroscopy on the lattice

Lattice QCD is very good at computing Euclidean (time-slice) correlation functions (CFs)

$$C(t) \;=\; \left\langle O(t)\, O^\dagger(0) \right\rangle \overset{\text{path int. repr.}}{\Longleftrightarrow} \langle\, \Omega \,|\, O(t)\, \hat{O}^\dagger(0) \,|\, \Omega \,\rangle$$

where the "operator" O is a (temporally) local combination of fields and $|\Omega\rangle$ the vacuum state

- Judiciously designed operators $O^\dagger$ create states of interest

$$O \;=\; O\left[\overline{\psi}(t), \psi(t), U(t)\right]$$

- Above path integral expression for $C(t)$ is related to an underlying QFT with Hamiltonian $\mathbb{H}$ and complete set of states $|n\rangle$:

$$\mathbb{H}|n\rangle \;=\; E_n|n\rangle \qquad\qquad \langle n|m\rangle \;=\; \delta_{nm} \qquad\qquad \textstyle\sum_n |n\rangle\langle n| \;=\; \mathbb{1}$$

- An important consequence of this connection is the "spectral decomposition" that allows extracting the (finite-volume) **energy eigenstates** from $C(t)$ acc. to

$$\left\langle O(t)\, O^\dagger(0) \right\rangle \;=\; \sum_n |c_n|^2\, \mathrm{e}^{-E_n t}$$

with matrix elements called **overlaps**

$$c_n \;=\; \langle\, n \,|\, \hat{O}^\dagger \,|\, \Omega \,\rangle$$

Symmetries

Consider:

A change of variables, under which the action of the theory is invariant, s.th.

$$\left\langle O(t)\, O^{\dagger}(0)\right\rangle \;=\; \left\langle O'(t)\, O'^{\dagger}(0)\right\rangle$$

- In QFT this means that some operator $\mathbb{U}$ commutes with $\mathbb{H}$
  $\rightarrow$ Energy eigenstates can be chosen to be also eigenstates of $\mathbb{U}$

$$\mathbb{H}|n\rangle \;=\; E_n|n\rangle \quad\Rightarrow\quad \mathbb{U}\mathbb{H}|n\rangle \;=\; E_n\mathbb{U}|n\rangle \quad\Rightarrow\quad \mathbb{H}\underbrace{\mathbb{U}|n\rangle}_{=|n\rangle'} \;=\; E_n\underbrace{\mathbb{U}|n\rangle}_{=|n\rangle'}$$

- If $|n\rangle \neq |n\rangle'$, we have a degeneracy of eigenstates

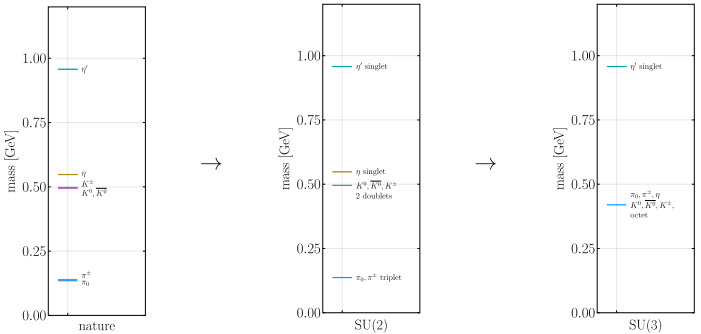
- If O is chosen carefully, then $\hat{O}^{\dagger}|0\rangle$ is an eigenstate of $\hat{U}$ and orthogonal to all states in different symmetry channels
  $\Rightarrow$ $c_n = 0$ for all $|n\rangle$ of a different symmetry channel than O

Symmetries: Flavour

Nature has no exact flavour symmetry, but an approximate SU(2), or even SU(3);
e.g., $N_f = 3 + 1$ QCD (we'll come back to it later) obeys

$$\begin{pmatrix} u \\ d \\ s \end{pmatrix} \to V \begin{pmatrix} u \\ d \\ s \end{pmatrix} \qquad (\bar{u}, \bar{d}, \bar{s}) \to (\bar{u}, \bar{d}, \bar{s})\, V^\dagger \qquad V \in \mathrm{SU}(3)$$

Symm. trafo leaves the action invariant $\Rightarrow$ Energy eigenstates can be labeled by $|D, Y, I, I_3\rangle$



Tackling excited states

Well-proven method is to solve a GEVP = Generalized Eigenvalue Problem $\longrightarrow$ Recipe:

[Michael & Teasdale, 1983, Lüscher & Wolff, 1990; Blossier at al., 2009]

- Assume we have several operators for the same symmetry channel, i.e. $O_1, O_2, \ldots, O_{N_{\text{op}}}$
- Compute a correlation matrix with elements $C_{ij}(t) = \left\langle O_i(t)\, O_j^\dagger(0) \right\rangle$
- Then the **generalised eigenvalues** $\lambda_n(t, t_0)$ solving the GEVP equation

$$C(t)V_n \;=\; \lambda_n\, C(t_0)V_n \qquad \text{behave as} \qquad \lambda_n(t,t_0) \;=\; \mathrm{e}^{-(t-t_0)E_n} \times \left\{1 \,+\, \mathrm{e}^{-(t-t_0)\Delta_n}\right\}$$

But then a variational basis with operators that have "good" (= large) **overlaps**

$$\langle\, n \,|\, \hat{O}_i^\dagger \,|\, \Omega \,\rangle \;\propto\; [\; C(t_0)V_n(t,t_0)\;]_i$$

with all states is required $\longrightarrow$ Excited spectra: large bases of operators with appropriate structures

The cubic group

Quantum numbers J^{PC} of states are defined by their transf. behaviour, where P and C are unaffected by discretisation, while J is related to dimension of an irreducible representation (irrep) of SO(3)

- Rotations on the lattice are characterised by the **cubic group** $O \simeq S_4$
- Subduced representations are known; J is now no longer unique

J	Dimension	Representation
0	1	A_1
1	3	T_1
2	5	$E \oplus T_2$
3	7	$A_2 \oplus T_1 \oplus T_2$
4	9	$A_1 \oplus E \oplus T_1 \oplus T_2$
...		

Table: Mapping to irreducible SO(3) representations

[e.g.: Lacock et al., 1996]

Lattice group irrep	J^{PC}	Meson operator
T_1^{--}	$1^{--}, 3^{--}, 4^{--} \ldots$	$\bar{q}_b \gamma_i q_a$
		$\bar{q}_b \gamma_4 \gamma_i q_a$
		$\bar{q}_b \overrightarrow{\nabla}_i q_a$
		$\bar{q}_b \overleftarrow{\nabla}_i \gamma_i \overrightarrow{\nabla}_i q_a$
		$\bar{q}_b \overleftarrow{\nabla}_i \gamma_4 \gamma_i \overrightarrow{\nabla}_i q_a$
		$\bar{q}_b \overleftarrow{\Delta} \overrightarrow{\nabla}_i q_a$
		$\bar{q}_b \epsilon_{ijk} \gamma_j \gamma_5 \overrightarrow{\nabla}_k q_a$
		$\bar{q}_b \overleftarrow{\Delta} \epsilon_{ijk} \gamma_j \gamma_5 \overrightarrow{\nabla}_k q_a$
A_1^{+-}	$0^{-+}, 4^{-+} \ldots$	$\bar{q}_b \gamma_5 q_a$
		$\bar{q}_b \overleftarrow{\nabla}_i \gamma_5 \overrightarrow{\nabla}_i q_a$

Table: Interpolators belonging to different irreps

[Mohler, Prelovsek & Woloshyn, 2013]

Illustration

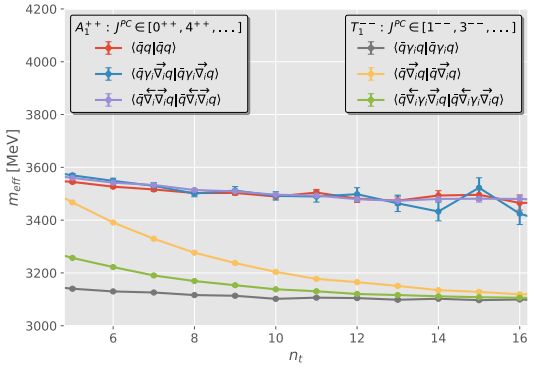


Figure: $N_f = 2$ example of effective masses from charmonium CFs decaying to ground state with n_t (this state is different for each irrep, and different operators decay at different rates)

$$\langle O_i(t)\, O_j^\dagger(0) \rangle = \sum_n |c_n|^2 \exp(-E_n t)$$

- **Isolate channel** with given lattice group representation of interest
- Parity controlled by γ_5 in the operator; charge given by exchange of $q \leftrightarrow \bar{q}$; many ops. known for each transf. behaviour
- We want **good overlap** with physical states of interest (typically the ground state)
- For that one needs **smooth** and **pysically extended** sources
  $\rightarrow$ Quark fields are often **smeared**

Smearing

For instance:

$$\langle O(t) O^{\dagger}(0) \rangle \;=\; \langle \bar{q}_1 \Gamma q_2 \, \bar{q}_2 \bar{\Gamma} q_1 \rangle$$

The correlator (expectation value) is the **trace** over a diagram such as

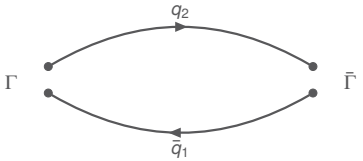
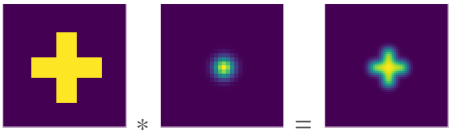


Figure: Sketch of the correlator; time is on x-axis; Γ fixes quantum numbers J^{PC} of particle states

- One can start from a point-source and ...
- ... usually prefers an iterative procedure

- $\bar{q}\,\Gamma\,q$ might have spatial component
- States are extended
  $\Rightarrow$ operators (interpolators) should be, too
- Interpolators must be **gauge invariant**
- (invariant source) $\bigotimes$ (covariant operation) = (new invariant source)



- This is a kind of **convolution**

Smearing

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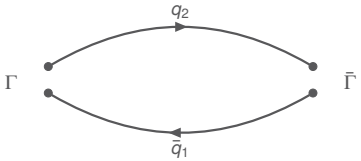

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Gaussian smearing

$$q_{n+1} \;=\; c_1\,(\mathbb{1} + c_2 H)\,q_n \qquad \text{with} \qquad H \;=\; \sum_i U_i(x)\delta_{x,y-i} \;+\; U_i^\dagger(x-i)\delta_{x,y+i}$$

- This iterative prescription acts only on nearest neighbours ...
- ... and approaches a convolution ($q_{\text{final}} = f * f * f \cdots f * q_{\text{initial}}$) with a **Gaussian**, by virtue of the central limit theorem
- c_2 and number of iterations control the shape
- Smooth shapes have generally better overlap with desired states
- There is a link between the scales of the source and the state
- **Note:** Dirac operator D needs to be re-inverted for each field

Distillation

Let's come back to the previous type of smearing

$$q_{n+1} \;=\; c_1\,(\mathbb{1} + c_2 H)\,q_n \qquad \text{with} \qquad H \;=\; \sum_i U_i(x)\delta_{x,y-i} \;+\; U_i^\dagger(x-i)\delta_{x,y+i}$$

The $d = 3$ (gauge-covariant) Laplacian is

$$\Delta(x,y) \;=\; \frac{1}{6} H(x,y) \;-\; \delta_{x,y}$$

Its repeated application to a quark field

$$q_n \;=\; \left(\mathbb{1} + \frac{\sigma}{n}\Delta\right)^n q_0 \qquad \Longrightarrow \qquad \lim_{n\to\infty} q_n \;=\; \mathrm{e}^{\sigma\Delta} q_0$$

thus leads to a suppression of higher **Laplacian eigenmodes**

Standard distillation

Observation: Higher eigenmodes of Δ suppressed $\Rightarrow$ Smearing fct. = Projector to "small space"

- Compute eigenvectors of the Laplacian and write quark fields in space of N_V **lowest eigenmodes**

  [M. Peardon et al., PRD 80 (2009) 054506]

$$q \;\rightarrow\; VV^\dagger q \qquad \text{with} \qquad \Delta V_i \;=\; \lambda_i V_i$$

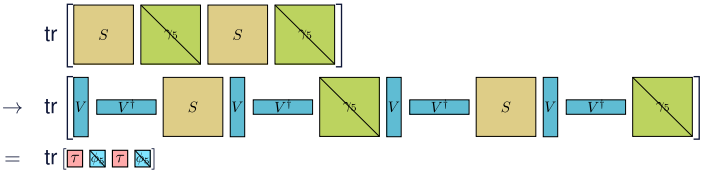
  where λ_i and V_i are eigenvalues and eigenvectors of the ($d = 3$ lattice) Laplacian Δ

- Properties (Pros & Cons):
  - $VV^\dagger$ is projector onto space of smooth, low-energy fields; trace evaluated in this space
  - Implies: Eigenmodes of Δ above certain index N_V are cut off, all lower ones used equally
  - Many inversions of D required, but they can be **pre-computed** and stored
  - Operators with distilled fields overlap largely onto low-lying states, but computational effort ($\propto N_V$) scales with spatial volume ($\Rightarrow$ more costly than other methods)

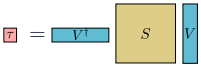
$\rightarrow$ Flexible method, increasingly being used for LQCD studies in hadron spectroscopy, etc.

Standard distillation

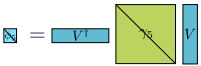
Example: One-meson $\langle PP \rangle$ correlator



With the **perambulator**
($\ni$ propagators $S \equiv D^{-1}$):



And the **elemental**:



[graphics by T. Korzec]

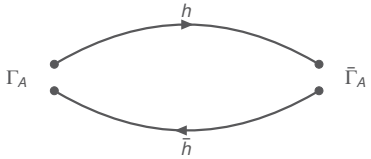


Figure: Sketch of the correlator; time is on x-axis

Distillation profiles

We can exploit the fact that one is free to choose [F. Knechtli et al., PRD 106 (2022) 034501]

$$q \quad \rightarrow \quad V J V^{\dagger} q$$

instead of $q \rightarrow V V^{\dagger} q$

- J is diagonal matrix with entries $g(\lambda_i)$, the **quark profile** (= function of Laplacian EVs)
- In practice: **Gaussians** are used for $g(\lambda_i)$
- Provides degree of freedom analogous to smearing
- Changes are **independent of inversion**, i.e., perambulators not affected (none of the inversions of the Dirac operator D must be re-done)
- The **optimal profile** is determined by solving the GEVP

Distillation profiles (a bit more explicit)

Distillation operator : $V(t)\,\mathbf{J(t)}\,V^\dagger(t)$

with V the eigenvectors of the lattice Laplacian; a common (= "standard") choice is $\mathbf{J} = \mathbb{1}$

Instead, parametrise the diagonal matrix $\mathbf{J}$ as

$$J^{\ i,j}_{\alpha,\beta}(t) \;=\; \delta_{ij}\,\delta_{\alpha\beta}\,\mathbf{g}(\lambda_\mathbf{i}(\mathbf{t})) \qquad\qquad \mathbf{g}(\lambda_\mathbf{i}): \quad \text{fcts. of Laplacian EVs}$$

thus providing an additional d.o.f. to be exploited in a variational formulation

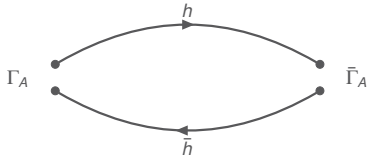
When calculating correlators, introduce the **perambulator** as before

$$\tau(t_1,t_2) \;=\; V^\dagger(t_1)\,D^{-1}\,V(t_2)$$

The rest is encoded in the **elemental**, now also incorporating the **quark profile** $\mathbf{g}(\lambda_\mathbf{i}(\mathbf{t}))$:

$$\Phi^{\ i,j}_{\alpha,\beta}(t) \;=\; V_i^\dagger(t)\,\Gamma_{\alpha,\beta}(t)\,\mathbf{g}^*(\lambda_\mathbf{i}(\mathbf{t}))\,\mathbf{g}(\lambda_\mathbf{j}(\mathbf{t}))\,V_j(t) \qquad [\,\Gamma = \text{generic combination of } \gamma\text{'s}\,]$$

Distillation profiles (a bit more explicit)



A meson 2-point correlation function then reads:

$$C(t) \;=\; -\left\langle \mathrm{tr}\left[\Phi_2(t)\,\tau_{q_a}(t,0)\,\bar{\Phi}_1(0)\,\tau_{q_b}(0,t)\right]\right\rangle_{\mathrm{gauge}}$$

- Choose *basis* of profiles: $g_n(\lambda) \;=\; \exp\left(-\frac{\lambda^2}{\sigma_n^2}\right)$ $\leftrightarrow$ **Gaussians** are beneficial choice
  - via $\mathbf{J} \neq \mathbb{1}$, higher eigenmodes are still cut off, but even below threshold the entries approaching N_V from below are suppressed
  - Extent of suppression is determined by the widths σ_n of the Gaussian profiles
- Optimise Φ via solving a GEVP that involves a suitable interpolator together with these basis profiles (now to be understood as different operators)
- Results in **"optimal" profile**: optimised lin. comb. $f = \sum_n c_n\, g_n^*\, g_n$ for any given state

Distillation profiles: Demonstration

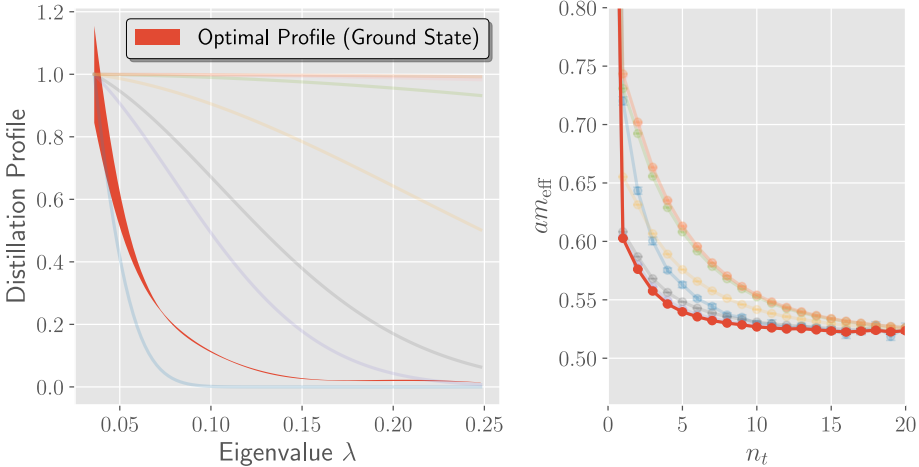


Figure: Example for heavy-light meson (left: profiles; right: effective mass, which shows faster approach to flat effective energies after solving the GEVP for the optimal profile)

Note: lower $\lambda \Leftrightarrow$ contributions from smoother fields, higher $\lambda \Leftrightarrow$ more localised sources

Performing the contractions

$$\langle\langle tr\left[\Phi_0(0)\tau_{q_0}(t_0,t_1)\Phi_1(t_1)\tau_{q_1}(t_1,t_2)\cdots\Phi_{N-1}(t_{N-1})\tau_{q_{N-1}}(t_{N-1},t_0)\right]\rangle\rangle_{\text{gauge}}$$

- τ and Φ are $4N_V \times 4N_V$ matrices
- Φ decomposes into $(4\times 4)\bigotimes(N_V \times N_V)^*$
- Changing the profiles ...
  - ... is volume independent
  - ... can be done independently for every t_n-combination

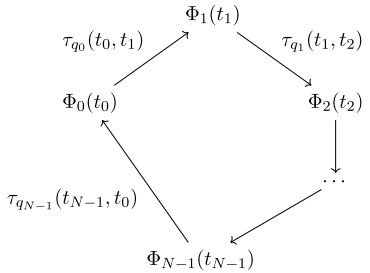


Figure: N-point diagram with distillation

Performing the contraction (pictorial notation)

$$\langle\langle tr\left[\blacksquare_0(0)\blacksquare_{q_0}(t_0,t_1)\blacksquare_1(t_1)\blacksquare_{q_1}(t_1,t_2)\cdots\blacksquare_{N-1}(t_{N-1})\blacksquare_{q_{N-1}}(t_{N-1},t_0)\right]\rangle\rangle_{\text{gauge}}$$

- $\blacksquare$ and $\blacksquare$ are $4N_V \times 4N_V$ matrices
- $\blacksquare$ decomposes into $(4\times 4)\bigotimes(N_V \times N_V)$
- Changing the profiles ...
  - ... is volume independent
  - ... can be done independently for every t_n-combination

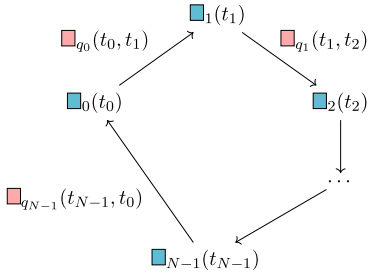


Figure: N-point diagram with distillation

Ensembles: $N_f = 2$ and $N_f = 3 + 1$

id	N_f	a [fm]	$L^3 \times T$	m_π [MeV]	N_V	N_{cnfg}
D5	2	0.0653	$24^3 \times 48$	439	200	150

- Wilson fermion action with non-perturbatively determined clover (= O(a)) improvement + plaquette gauge action [CLS; P. Fritzsch et al., NPB 865 (2012) 397; J. H. et al., PoS LATTICE2013 (2014) 475]
- Study to compute $\psi(3770) \longrightarrow \bar{D}D$ decay width [T. San José, B. Blossier, J. Neuendorf & J. H. @ Lattice 2024]

id	N_f	a [fm]	$L^3 \times T$	m_π [MeV]	N_V^{light}	N_V^{charm}	N_{cnfg}
A1h	3+1	≈ 0.069	$32^3 \times 96$	≈ 800	200	200	≈ 2000
A1	3+1	≈ 0.054	$32^3 \times 96$	≈ 420	100	200	≈ 4000

- Wilson fermion action with non-perturbatively determined clover (= O(a)) improvement + Lüscher-Weisz (= tree-level improved) gauge action; *physical* charm quark mass

[P. Fritzsch et al., JHEP 06 (2018) 025; R. Höllwieser et al., EPJC 80 (2020) 4]

- A1h and A1 have light quark masses at the SU(3)-symmetric point
- Control over decay thresholds (e.g., A1h: glueball $\longrightarrow \pi\pi$; A1: glueball $\longrightarrow \pi\pi, \pi\pi\pi\pi$)

Charmonium spectroscopy

Example on D5 ($N_f = 2$, 48×24^3):

- We are interested in $\psi'' \equiv \psi(3770)$ (2nd excited $c\bar{c}$ state, 1^{--})

  [J. Neuendorf et al. @ Lattice 2024]

- Solving an (8×8)–GEVP with:
  - Operators with γ_i and $\gamma_4\gamma_i$ in Dirac space
  - Different smearing levels
  - Including operators with covariant derivatives

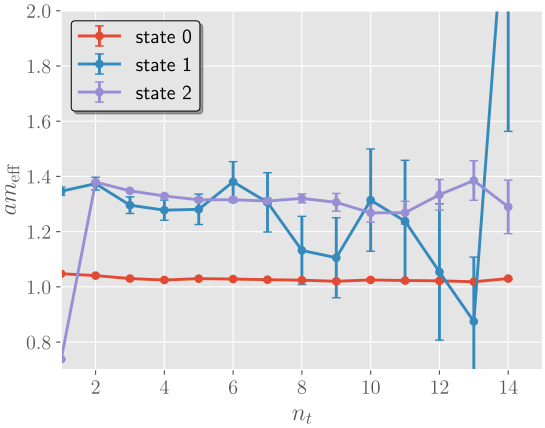


Figure: Spectrum of vector charmonium **without** distillation

Charmonium spectroscopy

Example on D5 ($N_f = 2$, 48×24^3),
now **with distillation:**

- We are interested in $\psi'' \equiv \psi(3770)$
  (2nd excited $c\bar{c}$ state, 1^{--})

  [J. Neuendorf et al. @ Lattice 2024]

- Solving an (14×14)–GEVP with:
  - Operators with γ_i and $\gamma_4\gamma_i$
    in Dirac space
  - Different profiles
  - **No** covariant derivative ops.

  $\Rightarrow$ **Correct state identification**

- Similar dependence on γ_4 inclusion

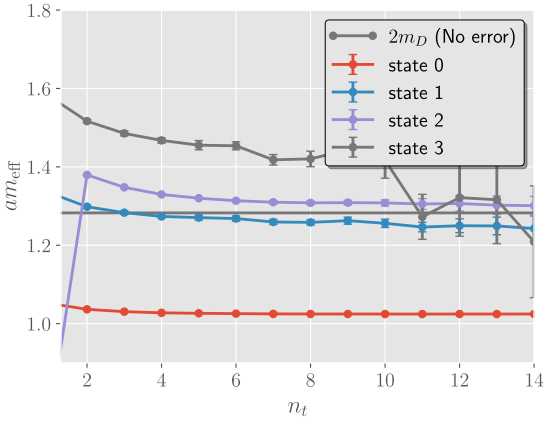


Figure: Spectrum of vector charmonium **with** distillation

Charmonium spectroscopy

Example on D5 ($N_f = 2$, 48×24^3),

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- We are interested in $\psi'' \equiv \psi(3770)$ (2^{nd} excited $c\bar{c}$ state, 1^{--})

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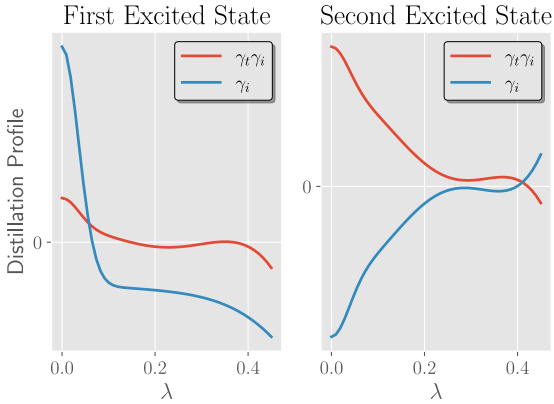


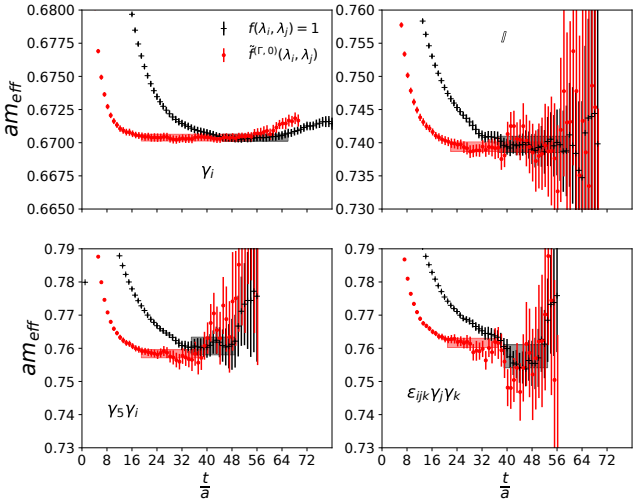
Figure: Optimal distillation profiles

Charmonium spectroscopy

[J.A. Urrea-Niño, J. Finkenrath, R. Höllwieser, F. Knechtli, T. Korzec & M. Peardon]

Another example: Ongoing study with distillation profiles close to the physical point

- $N_f = 3 + 1$
- $48^3 \times 144$, $a \approx 0.043\,\mathrm{fm}$
- SU(3) flavour-symmetric quark mass point, physical charm
- Method of optimal distillation profiles reduces excited-state contamination at early times
- Even more marked improvement obtained w.r.t. to std. distillation



D and D^* mesons

Comparison of different meson channels, including D and D^* mesons:

- Different particles show different optimal profiles
- Charmonium wider than D, D wider than π
- Narrower profile
  $\Leftrightarrow$
  Less localised contributions
- Different shapes for excited states (not shown here)

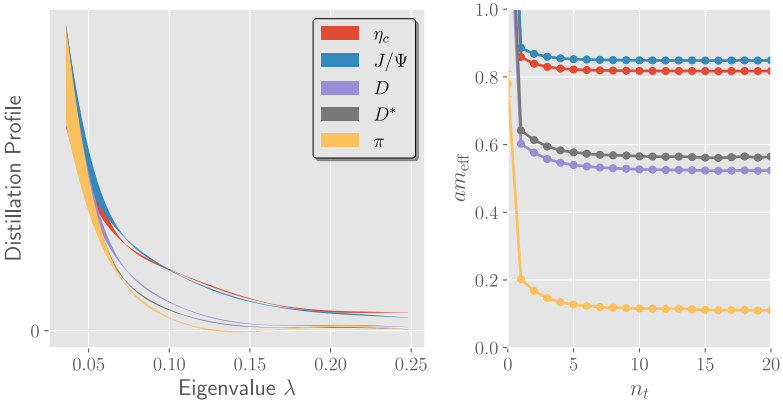


Figure: Different profiles and masses on A1 ensemble ($N_f = 3 + 1$)

Distillation profiles in real space

Illustration follows

[F. Knechtli et al., PRD 106 (2022) 034501]

- Reconstructed operator **applied to a point source**
- Take **spatial slice** and average over n_t and configurations
- tr $[\gamma_5 \Gamma]$ and colour average yield **scalar value**
- D displays more significant less-localised background
- Rings indicate excited states

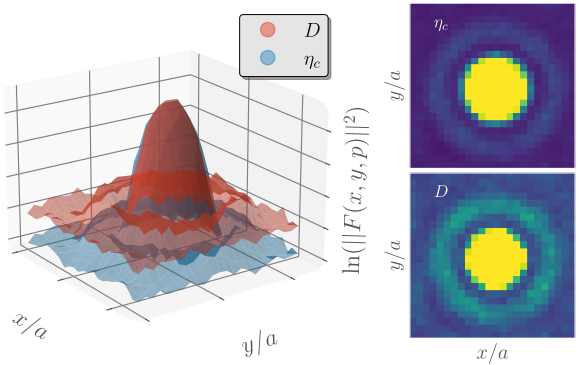
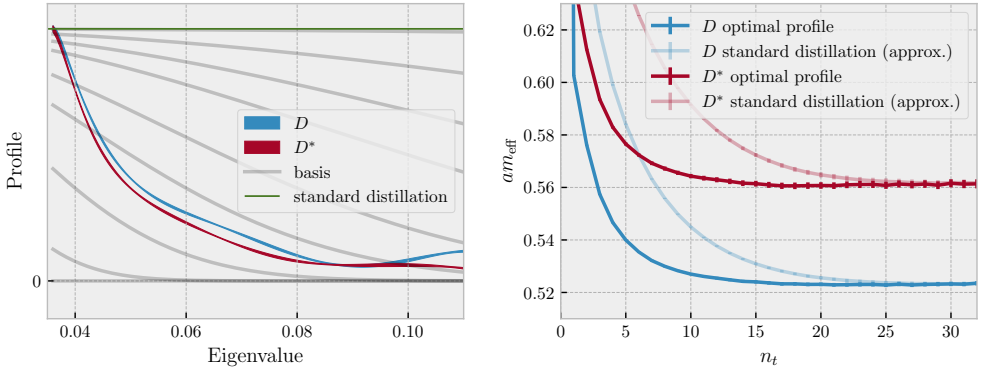


Figure: Optimal profiles in real space ($N_f = 2$ ensemble D5)

D and D^* mesons

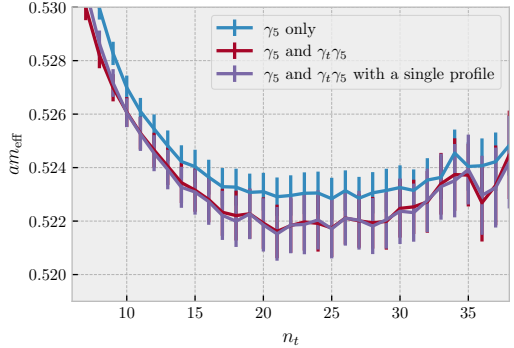
Optimal $D^{(*)}$-Profiles

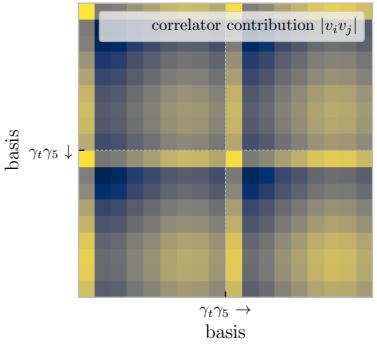


- Comparison between optimal distillation profiles and standard distillation on A1 (the latter is almost perfectly approximated by the widest profile)
- L.h.s.: 9 basis profiles, $N_V = 100$; higher EVs not shown on x-axis, as they have small impact
- General observation: at $N_V = 100$, *standard* distillation plateaus not only develop later, but also never become as good as the *optimised* profile (see also static-light case)

D and D^* mesons

Mixing Profiles and γ-Structure





- Test of including $\gamma_t\gamma_5$ operators for the D and its effect on ground-state plateau quality
- R.h.s.: colour coding of matrix entries indicates absolute value of the resp. contribution to the GEVP solution for the optimal profile
- Slight improvement (?), but it doesn't matter if one solves for the optimal "total" profile (via a 18×18 GEVP) or re-using the profile of the γ_5 operators on the $\gamma_t\gamma_5$ ones (via a 9×9 GEVP)

Profiles and momenta

Distillation profiles may also be incorporated in **correlators with non-zero lattice momenta**

Elementals with lattice momentum
(Dirac indices of Γ suppressed) ...

$$\Phi_{i,j}(\vec{p}) \;=\; \sum_{\vec{x}} V_i^{\dagger}(\vec{x})\, \mathrm{e}^{-i\,\vec{p}\cdot\vec{x}}\, g^{*}(\lambda_i)\, g(\lambda_j)\, \Gamma\, V_j(\vec{x})$$

... can be split s.th. part encoding the momentum can be *pre-calculated*:

$$\Phi_{i,j}(\vec{p}) \;=\; \Gamma g(\lambda_i) g(\lambda_j) \sum_{\vec{x}} V_i^{\dagger}(\vec{x})\, \mathrm{e}^{-i\,\vec{p}\cdot\vec{x}}\, V_j(\vec{x})$$

→ This is the only additional cost, because the perambulators are unaffected and *no repeated inversions* are needed

Alternative way to induce momentum:
Partially twisted periodic boundary conditions

[Sachrajda & Villadoro, PLB 609 (2005) 73]

- Inversion with
  $\psi(x+L) = \mathrm{e}^{i\,\theta}\psi(x)$
  $\Longrightarrow\; p = \frac{2\pi n+\theta}{L}$
- Allows **continuos momenta**
- Requires *new inversions*

Profiles and momenta

Distillation profiles may also be incorporated in **correlators with non-zero lattice momenta**

- Different momenta exhibit different optimal profiles
- Profiles still improve results
- Using profiles works with both ways of implementing lattice momenta

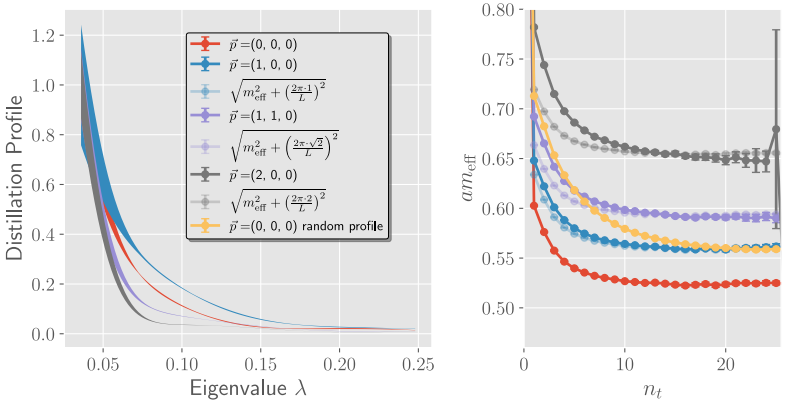


Figure: Opt. profiles and energies at different momenta on A1 ($N_f = 3 + 1$)

Profiles and momenta

Distillation profiles may also be incorporated in **correlators with non-zero lattice momenta**

- Different momenta exhibit different optimal profiles
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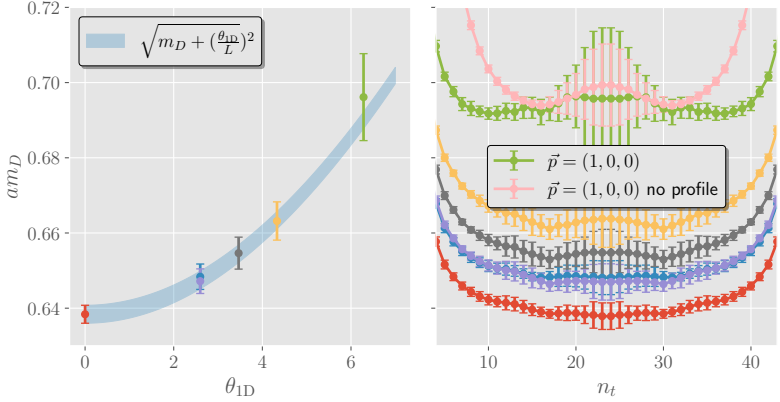
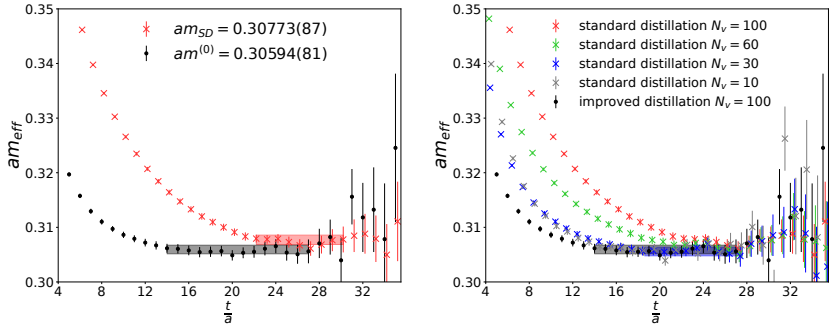


Figure: Both methods fulfill **dispersion relation** (here for D5, $N_f = 2$); profiles are effective at higher momenta [J. Neuendorf @ Lattice 2023]

Further applications: The static-light system

[L. Struckmeier, R. Höllwieser, F. Knechtli, T. Korzec, M. Peardon & J.A. Urrea-Niño; talk by L. S. @ Lattice 2024]

- Investigate optimised distillation for static-light = *static limit of B mesons* / LO of HQET
  → e.g., helpful for quantifying excited-state contamination in B correlators ($B\pi$ system)
- Study on $N_f = 3 + 1$ ensembles: Distillation profiles lead to improvement also in this case



- Left: $N_V = 100$; high supression of excited-state contamination through optimal profiles
- Right: Std. dist. very sensitive to N_v, **impr. dist. profiles make best use of available vectors**

Further applications: The static-light system

[L. Struckmeier, R. Höllwieser, F. Knechtli, T. Korzec, M. Peardon & J.A. Urrea-Niño; talk by L. S. @ Lattice 2024]

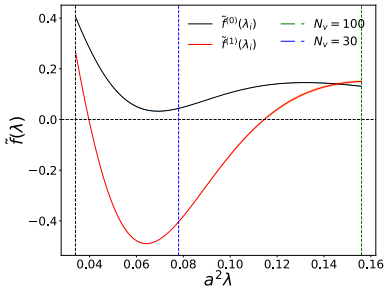


Figure: A1 ensemble.

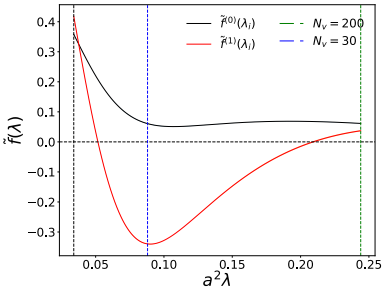


Figure: A1h ensemble.

Optimal meson profiles:

- The higher the state, the more structure in the optimal profile
- Larger eigenvalues still have non-negligible contribution
- Larger eigenvalues needed for excited states [first static-light / static-charm spectrum results exist]

Summary & Outlook

- Investigations reveal the efficacy of distillation profiles across a range of scenarios, particularly demonstrating their merit also for heavy-light systems

- Profiles tend to become narrower for lighter particles (i.e., when lighter quarks are included) and therefore have better overlap with more smeared sources
  $\rightarrow$ Restricting the number of light eigenmodes is possible to save computation cost

- Moreover, optimal profiles can also be obtained for CFs with (different types of) **non-zero lattice momenta**
  $\rightarrow$ Combine: more complex diagrams + momenta + profiles

  [J. Neuendorf et al., PoS LATTICE2023 (2024) 057; work in progress @ U. Münster & U. Wuppertal]

- Another direction of application (not discussed today):
  Mixing of flavours, glueballs and 2-pion states in the scalar channel

  [J.A. Urrea-Niño et al., talk by J.A. U.-N. @ Lattice 2024; work in progress @ U. Wuppertal & TCD]

Summary & Outlook

- Among the physical goals: address decays involving $D^{(*)}$ mesons, such as $\psi(3770) \to D\bar{D}$ or $T_{cc} \to DD^*$
  (via a scattering analysis on the lattice based on the Lüscher formalism)

- Intermediate target: study DD^* scattering in the $J^{PC} = 1^{++}$ ($I = 0$) channel
  $\to$ Is there evidence for a charmonium-like state $X(3872)$ below the $D\bar{D}^*$ threshold?

  [cf. earlier studies by S. Prelovsek et al, 2013 & 2015]

  $\to$ Explore excited charmonium spectrum in this channel
  $\to$ Estimate $m_{\chi_{c1}}(2P) - (m_D + m_{D^*})$ on our lattices, ...

- For this, as a first step, we are currently trying to find optimal profiles in correlation functions of **two-meson operators**, to be included in the GEVP, such as