

Bachelor thesis

Computation of meson correlation functions using distillation: Computation of correlators

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Abstract

This work describes the computation of meson correlation functions via distillation for Wilson twisted mass fermions and its implementation. Correlation functions for charmonium states are calculated on 11 gauge configuration on a $24^3 \times 48$ sized lattice using 1, 2, 5 and 10 eigenvectors of the lattice Laplacian.

Contents

1	Introduction	2
2	Theoretical basics	3
2.1	QCD	3
2.2	Lattice QCD	3
2.3	Wilson twisted mass QCD	4
2.4	Meson correlation functions	5
2.4.1	Creation operators	5
2.4.2	Meson correlation functions	5
3	Distillation	8
3.1	Distillation operator	8
3.2	Smearing behaviour of distillation	9
3.3	Distilled meson two-point correlation functions	9
3.4	Computation of the perambulator	10
4	Implementation	12
4.1	Overview	12
4.2	Programs	12
4.2.1	Computation of the perambulators	12
4.2.2	Computation of the distilled gamma matrix	13
4.2.3	Computation of the correlation function	13
4.2.4	Python control script	13
5	Results	14
5.1	Lattice setup	14
5.2	Meson masses	14
6	Discussion	16
6.1	Complexity of the simulation depending on the number of eigenvectors	16
6.2	Outlook	17
7	References	18

1 Introduction

Computing masses of the particles in the Standard Model and investigating the force between them is subject of many thesis and papers and will be the topic of many to come. This work focuses on particles interacting via the strong force and hence utilizes the theory of QCD. The elementary particles of QCD are called quarks which come in six flavors. Gluons on the other hand are the exchange particles of the strong force. Gluons are massless bosons and carry a color charge similar to the quarks.

Hadrons are particles consisting of quarks and one distinguishes between mesons, hadrons composed of a quark-antiquark pair, and baryons which are bound states of three quarks. Physical properties of hadrons arise from the dynamics of the theory. These properties such as mass and electrical charge can be experimentally tested. It is therefore crucial for an elementary theory like QCD to reproduce these measurements to certain precision.

Computing observables of QCD can usually only be achieved by a numerical treatment. One theory to treat QCD on computers is called *lattice QCD*. In *lattice QCD* one defines a finite space-time lattice composed of a series of discrete points. On such lattices the masses of mesonic states can be obtained from so called correlators which are vacuum expectation values of hadron creation operators. These correlators can be numerically computed and the mass is extracted by an exponential fit.

When finding suitable creation operators in such a way that they generate the quantum numbers of interest one has some degrees of freedom constructing them. This freedom is used by a method called *distillation* which describes a way to construct hadron creation numbers using eigenvectors of the lattice laplacian.

This thesis describes a first test implementing the computation of meson correlation functions using distillation in our work group and the results this implementation yielded.

2 Theoretical basics

Throughout this work natural units will be used, so that $\hbar = c = a = 1$, where a is the distance between two lattice points. In any instance where one index appears twice the **Einstein summation notation** was used, an implicit summation is assumed. When working with path integrals the euclidean formulation of QCD is used where the real time x_0 is replaced with the imaginary time $x_0 = -ix_4$. Therefore the Minkowsky tensor $g_{\mu\nu}$ is replaced by $\delta_{\mu\nu}$.

2.1 QCD

Quantum chromodynamics is a $SU(3)$ gauge quantum field theory and describes quarks and gluons. The QCD Lagrangian is defined as [10]

$$\mathcal{L}_{QCD}[\psi, \bar{\psi}, A] = \sum_f \bar{\psi}_f(x)(\gamma_\mu \mathcal{D}_\mu + m_f)\psi_f(x) + \frac{1}{4}F_{\mu\nu}^a F_{\mu\nu}^a. \quad (1)$$

$\psi(x)$ represents the quark field, $\mathcal{D}_\mu = \partial_\mu - igA_\mu(x) = \partial_\mu - igT^a A_\mu^a(x)$ is the gauge covariant derivative and $F_{\mu\nu} = T^a F_{\mu\nu}^a$ is the field strength tensor of the theory. The latter is defined as

$$\begin{aligned} F_{\mu\nu} &= \partial_\mu A_\nu - \partial_\nu A_\mu - ig[A_\mu, A_\nu] \\ &= T^a(\partial_\mu A_\nu^a - \partial_\nu A_\mu^a + gf^{abc}A_\mu^b A_\nu^c). \end{aligned} \quad (2)$$

The T^a 's are called $SU(3)$ generators and are part of the $SU(3)$ Lie algebra with the commutator relationship $[T^a, T^b] = if^{abc}T^c$. The action is given by

$$S_{QCD}[\psi, \bar{\psi}, A] = \int d^4x \mathcal{L}_{QCD}[\psi, \bar{\psi}, A] \quad (3)$$

and is invariant under local $SU(3)$ transformations. It is also invariant under $U(1)$ transformations. The first term of the lagrangian and hence the action displays information about the dynamic of the theory, the second term about the self interaction of the gluons.

The internal degrees of freedom of the quark fields ψ and $\bar{\psi} = \psi^\dagger \gamma_4$ separate into three parts: Spin (A), color (c) and flavor (f) with 4, 3, and N_f components respectively. The gluon fields have eight color degrees of freedom and transform under the adjoint representation of $SU(3)$.

2.2 Lattice QCD

In lattice QCD one defines a hypercubic, discrete spacetime lattice

$$\Lambda = \{x | \frac{|x^\mu|}{a} \in \{0, L_\mu\}\}, \mu = 1, 2, 3, 4 \quad (4)$$

where a is the lattice spacing and x^μ is a vector along the μ -axis of the lattice. The L_μ 's define the size of the lattice. Usually the spacial dimensions are chosen to be equal, so that $L_1 = L_2 = L_3 = L$. A finite lattice breaks the translational invariance of the theory which would violate momentum conservation. To eliminate this issue periodic boundary conditions are used

$$\mathbf{x} + L_\mu \hat{\boldsymbol{\mu}} = \mathbf{x} \quad (5)$$

where $\hat{\boldsymbol{\mu}}$ defines the unit vector along the μ -axis.

In lattice QCD the action has to be redefined replacing A_μ by so called link variables U_μ which preserve all symmetries of the action.

$$S_{QCD}[\psi, \bar{\psi}, A] \rightarrow S_{Lattice-QCD}[\psi, \bar{\psi}, U] \quad (6)$$

These link variables are elements of SU(3) algebra and are defined as

$$U_\mu(x) = e^{-igA_\mu(x)} \quad (7)$$

A closed loop of link variables is gauge invariant and the simplest one is called plaquette $U_{\mu\nu}$ [12]. A plaquette in the $\mu - \nu$ plane is defined by

$$U_{\mu\nu}(x) = U_\mu(x)U_\nu(x + \hat{\mu})U_\mu^\dagger(x + \hat{\nu})U_\nu^\dagger(x) \quad (8)$$

where the link variables are path ordered. The simplest formulation of the lattice action can be derived from this plaquette [3]

$$S_g[U] = \frac{6}{g^2} \sum_x \sum_{\mu < \nu} \text{ReTr} \frac{1}{3} (1 - U_{\mu\nu}) \quad (9)$$

For fermions we find as the simplest (called *naive*) action

$$\begin{aligned} S[\psi, \bar{\psi}, U] &= m_q \sum_x \bar{\psi}(x)\psi(x) \\ &+ \frac{1}{2a} \sum_x \bar{\psi}(x) \gamma_\mu [U_\mu(x)\psi(x + \hat{\mu}) - U_\mu^\dagger(x - \hat{\mu})\psi(x - \hat{\mu})] \\ &\equiv \sum_x \bar{\psi}(x) M_{xy}[U] \psi(x) \end{aligned} \quad (10)$$

Here $M_{xy}[U]$ is the lattice Dirac operator.

$$M_{ij}[U] = m_q \delta_{ij} + \frac{1}{2a} \sum_\mu \gamma_\mu (U_{i,\mu} \delta_{i,j-\mu} - U_{i-\mu,\mu} \delta_{i,j+\mu}) \quad (11)$$

For $m_q = 0$ the naive action (10) has both vector and axial symmetry, preserves chiral symmetry but introduces so called *fermion doubling* [3]. To prevent fermion doubling which is a pure lattice artifact one approach introduces additional mass terms, so called *Wilson fermions*.

2.3 Wilson twisted mass QCD

In twisted mass QCD a mass term is added to the action (10). For a field χ this term reads [13]

$$i\mu_q \bar{\chi} \gamma_5 \tau_3 \chi \quad (12)$$

τ_3 is the Pauli matrix in flavor space and μ_q is the twisted mass. In a *twisted basis* $\{\chi, \bar{\chi}\}$ the tmQCD action is

$$S_F[\chi, \bar{\chi}, A] = \int d^4x \bar{\chi} (\gamma_\mu \mathcal{D}_\mu + m_q + i\mu_q \gamma_5 \tau_3) \chi \quad (13)$$

The mass term can be written as $m_q + i\mu_q \gamma_5 \tau_3 = M e^{i\alpha \gamma_5 \tau_3}$. The *twisted basis* is a mere coordination transformation of the *physical basis* $\{\psi, \bar{\psi}\}$

$$\psi = e^{i\omega \gamma_5 \tau_3 / 2} \chi, \quad \bar{\psi} = \bar{\chi} e^{i\omega \gamma_5 \tau_3 / 2} \quad (14)$$

where ω is called the *twisted angle*. For $\alpha = \omega$ we obtain the standard QCD action. Using tmQCD fixes the extra degrees of freedom introduced by the naive action. It has its own problems, though: The τ_3 matrix switches the signes for up- and down-type quarks which breaks isospin conservation. The γ_5 matrix on the other hand implies that parity is no longer a symmetry.

2.4 Meson correlation functions

Mesons are quark-antiquark states which can be characterized by the following QCD quantum numbers [14]:

- Spin and total angular momentum $J = 0, 1, 2, \dots$ (all mesons are bosons)
- Parity $P = \pm 1$
- Charge conjugation $C = \pm 1$
- Flavor quantum numbers:
 - u and d : Isospin I ; $I_z = \pm \frac{1}{2}$
 - s and \bar{s} : Strangeness S ; $S = \pm 1$
 - c and \bar{c} : Charmness C ; $C = \pm 1$
 - b and \bar{b} : Bottomness B' ; $B' = \pm 1$
 - t and \bar{t} : Topness T ; $T = \pm 1$
- Electric charge will be neglected.

2.4.1 Creation operators

To examine a meson with a particular set of quantum numbers $I(J^P)$ one needs to define a corresponding creation operator $\mathcal{O}(x)$. When acting on the vacuum $\mathcal{O}(x)$ creates a so called trial state $|\phi, x\rangle$ with the quantum numbers $I(J^P)$ [14]:

$$\mathcal{O}(x)|\Omega\rangle = |\phi, x\rangle \quad (15)$$

Meson creation operators can be assembled in different ways, the easiest is

$$\begin{aligned} \mathcal{O}(x) &= \sum_x \bar{\psi}^{(f_1)}(x) \Gamma \psi^{(f_2)}(x) \\ \mathcal{O}^\dagger(x) &= \pm \sum_x \bar{\psi}^{(f_2)}(x) \Gamma \psi^{(f_1)}(x) \end{aligned} \quad (16)$$

Γ is a matrix in Dirac space which carries total momentum J and parity P . The sign in (16) depends on the choice of Γ because $\gamma_4 \Gamma^\dagger \gamma_4 = \pm \Gamma$. The following table lists the possible configurations for Γ :

Γ	J	P	Transformation
$1, \gamma_4$	0	+1	scalar
$\gamma_5, \gamma_4 \gamma_5$	0	-1	pseudoscalar
$\gamma_i, \gamma_4 \gamma_i$	1	-1	vector
$\gamma_4 \gamma_i$	1	+1	axial vector

Table 1: Possible configurations for Γ and corresponding quantum numbers

2.4.2 Meson correlation functions

To determine the energy of an eigenstate of the Hamiltonian of a quantum field theory one can calculate the vacuum expectation value (VEV) of the respective creation operator. Also called the correlator, the VEV can be computed by the Feynman path integral:

$$\begin{aligned} C(t_2 - t_1) &\equiv \langle \Omega | \mathcal{O}^\dagger(t_2) \mathcal{O}(t_1) | \Omega \rangle \\ &= \frac{1}{Z} \int D[\psi] D[\bar{\psi}] D[A] \mathcal{O}^\dagger(t_2) \mathcal{O}(t_1) e^{-S[\psi, \bar{\psi}, A]} \end{aligned} \quad (17)$$

where Z defines the partition function:

$$Z = \int D[\psi]D[\bar{\psi}]D[A] e^{-S[\psi,\bar{\psi},A]} \quad (18)$$

$S[\psi, \bar{\psi}, A]$ is the lattice action. Introducing a finite lattice spacing some difficulties calculating the path integral are solved. The integral becomes regularized and the infinite dimensional integral can be replaced by a finite product of finite dimensional integrals:

$$\int D[\psi]D[\bar{\psi}]D[A] \approx \prod_{x \in \Lambda} \int d\psi(x)d\bar{\psi}(x)dA(x) \quad (19)$$

To calculate the mesonic energy spectrum one introduces a complete set of energy eigenstates $\sum_k |k\rangle\langle k| = 1$ into equation (17):

$$C(t_2 - t_1) = \sum_k \langle \Omega | \mathcal{O}^\dagger(t_2) | k \rangle \langle k | \mathcal{O}(t_1) | \Omega \rangle \quad (20)$$

One can now exploit that $\mathcal{O}^\dagger(t_2)$ is a Heisenberg operator and its temporal evolution can be described by

$$\mathcal{O}^\dagger(t_2) = e^{H(t_2-t_1)} \mathcal{O}^\dagger(t_1) e^{-H(t_2-t_1)} \quad (21)$$

So we can write (20) as

$$\begin{aligned} C(t_2 - t_1) &= \sum_k \langle \Omega | e^{H(t_2-t_1)} \mathcal{O}^\dagger(t_1) e^{-H(t_2-t_1)} | k \rangle \langle k | \mathcal{O}(t_1) | \Omega \rangle \\ &= \sum_k \langle \Omega | e^{E_\Omega(t_2-t_1)} \mathcal{O}^\dagger(t_1) e^{-E_k(t_2-t_1)} | k \rangle \langle k | \mathcal{O}(t_1) | \Omega \rangle \\ &= \sum_k (\langle k | \mathcal{O}(t_1) | \Omega \rangle)^\dagger \langle k | \mathcal{O}(t_1) | \Omega \rangle e^{(E_\Omega - E_k)(t_2-t_1)} \\ &= \sum_k |\langle k | \mathcal{O}(t_1) | \Omega \rangle|^2 e^{-E(t_2-t_1)} \end{aligned} \quad (22)$$

where $E = E_k - E_\Omega$ is the energy of the energystate $|k\rangle$ relative to the vacuum energy.

One can, after calculating the path integral numerically, extract the meson mass by fitting an exponential curve to the correlation function. To compute the correlator numerically we use definition (16) where the integration over the fermion fields in lattice QCD can be done manually:

$$\begin{aligned} C(t_2 - t_1) &= \langle \Omega | \mathcal{O}^\dagger(t_2) \mathcal{O}(t_1) | \Omega \rangle \\ &= \pm \sum_{\mathbf{x}, \mathbf{y} \in \Lambda} \langle \Omega | \bar{\psi}^{(f_1)}(\mathbf{x}, t_2) \Gamma \psi^{(f_2)}(\mathbf{x}, t_2) \bar{\psi}^{(f_2)}(\mathbf{y}, t_1) \Gamma \psi^{(f_1)}(\mathbf{y}, t_1) | \Omega \rangle \\ &= \pm \sum_{\mathbf{x}, \mathbf{y} \in \Lambda} \langle \Omega | \bar{\psi}_A^{(f_1),a}(\mathbf{x}, t_2) \Gamma_{AB} \psi_B^{(f_2),a}(\mathbf{x}, t_2) \bar{\psi}_C^{(f_2),b}(\mathbf{y}, t_1) \Gamma_{CD} \psi_D^{(f_1),b}(\mathbf{y}, t_1) | \Omega \rangle \\ &= \mp \sum_{\mathbf{x}, \mathbf{y} \in \Lambda} \Gamma_{AB} \Gamma_{CD} \langle \Omega | \psi_D^{(f_1),b}(\mathbf{y}, t_1) \bar{\psi}_A^{(f_1),a}(\mathbf{x}, t_2) \psi_B^{(f_2),a}(\mathbf{x}, t_2) \bar{\psi}_C^{(f_2),b}(\mathbf{y}, t_1) | \Omega \rangle \end{aligned} \quad (23)$$

The \pm sign is introduced from the hermition adjoint (16) of the meson creation operator. In the last line we have an additional minus sign because we interchanged Grassmann valued fields three times.

Integration of the fermion fields can be done independently for each flavor and defines the Propagator $(D^{(f)})^{-1}(\mathbf{x}, t_2; \mathbf{y}, t_1)$ [7]:

$$\langle \psi_A^{(f),a}(\mathbf{x}, t_2) \bar{\psi}_B^{(f),b}(\mathbf{y}, t_1) \rangle_F = (D^{-1(f)})_{AB}^{ab}(\mathbf{x}, t_2; \mathbf{y}, t_1) \quad (24)$$

where $\langle \dots \rangle_F$ describes the fermionic expectation value. Therefore only the path integral over the gauge fields $\langle \dots \rangle_A$ weighted by $e^{-S_{eff}[A]}$ remains and equation (23) becomes:

$$\begin{aligned} C(t_2 - t_1) &= \mp \sum_{\mathbf{x}, \mathbf{y} \in \Lambda} \Gamma_{AB} \Gamma_{CD} \langle (D^{-1(f_1)})_{DA}^{ba}(\mathbf{y}, t_1, \mathbf{x}, t_2) (D^{-1(f_2)})_{BC}^{ab}(\mathbf{x}, t_2, \mathbf{y}, t_1) \rangle_A \\ &= \mp \sum_{\mathbf{x}, \mathbf{y} \in \Lambda} \langle (D^{-1(f_1)})_{DA}^{ba}(\mathbf{y}, t_1, \mathbf{x}, t_2) \Gamma_{AB} (D^{-1(f_2)})_{BC}^{ab}(\mathbf{x}, t_2, \mathbf{y}, t_1) \Gamma_{CD} \rangle_A \\ &= \mp \sum_{\mathbf{x}, \mathbf{y} \in \Lambda} \langle Tr[(D^{-1(f_1)})(\mathbf{y}, t_1, \mathbf{x}, t_2) \Gamma (D^{-1(f_2)})(\mathbf{x}, t_2, \mathbf{y}, t_1) \Gamma] \rangle_A \end{aligned} \quad (25)$$

The trace $Tr[\dots]$ acts in Dirac and in color space.

On a finite lattice the path integral in equation (25) is of finite dimension and can be done numerically. It is usually calculated by averaging over gauge field configurations which can be obtained using Monte Carlo methods.

Inverting the Dirac operator directly is close to impossible, it is represented by a very large quadratic matrix which has $L_1 \times L_2 \times L_3 \times T \times 3 \times 4$ complex entries. One method is the computation of so called point-to-all propagators [1] which describe the quark propagators from one point on the lattice to all others. This approach comes at a cost: A loss of physical information and large statistical errors.

3 Distillation

The term distillation describes a quark-field smearing algorithm to compute hadron correlation functions. It was first described in 2009 by Michael Peardon [9]. Distillation allows the computations of all-to-all quark propagators at reasonable cost.

3.1 Distillation operator

Smearing is a method to apply a smoothing function to the quark field before applying the creation operators. Smearing should remove short-range modes while respecting all symmetries. Distillation makes use of a gauge-covariant quark smearing based on the lattice laplacian which is defined as follows

$$-\nabla_{xy}^2 = 6\delta_{xy} - \sum_{j=1}^3 (\tilde{U}_j(x, t)\delta_{x+j, y} + \tilde{U}_j^\dagger(x - y, t)\delta_{x-j, y}) \quad (26)$$

Starting from the lattice Laplacian one can define a typical, conventional smearing by the following smearing operator

$$J_{\omega, n}(t) = \left(1 + \frac{\omega \nabla^2(t)}{n}\right)^n \quad (27)$$

where ω and n are tunable parameters. For large n , J defines the exponential of $\omega \nabla^2$ which suppresses higher eigenmodes of the laplacian, hence only a few of the lowest modes contribute to J .

$$\lim_{n \rightarrow \infty} J_{\omega, n}(t) = \exp(\omega \nabla^2) \equiv J_\omega \quad (28)$$

The lattice laplacian is a gauge-covariant, linear, negative-definite and hermitian operator acting on a M dimensional Hilbert space. On each timeslice its eigenvectors are orthogonal and one can find an orthonormal basis of \mathbb{C}^M [6]

$$\sum_{k=1}^M |v_k\rangle \langle v_k| = 1 \quad (29)$$

where v_k defines the k^{th} eigenvector on the corresponding timeslice.

$$\nabla^2 |v_k\rangle = \lambda_k |v_k\rangle \quad (30)$$

The eigenvalues of the lattice laplacian are semi-negative $\lambda_k \in (-\infty, 0]$ and we label them according to $\lambda_{k+1} < \lambda_k$.

Using the above we can now expand J_ω in the limit $n \rightarrow \infty$ using (29):

$$\begin{aligned} J_\omega &= \sum_{k=1}^M |v_k\rangle \langle v_k| J_\omega \\ &= \sum_{k=1}^M |v_k\rangle \langle v_k| \exp(\omega \nabla^2) \\ &= \sum_{k=1}^M |v_k\rangle \langle v_k| \exp(\omega \lambda_k) \end{aligned} \quad (31)$$

One can see that higher eigenmodes are suppressed exponentially. Therefore there is some number $N \ll M$ such that the remaining terms vanish, $\exp(\omega \lambda_k) \ll 1$ for $k > N$ holds. So we can write

$$J_\omega \approx \sum_{k=1}^N |v_k\rangle \langle v_k| \exp(\omega \lambda_k) \quad (32)$$

This motivates the definition of the distillation operator which is constructed by [9]:

$$\square_t \equiv V_t V_t^\dagger \quad (33)$$

V_t is a $M \times N$ matrix which k^{th} column contains the k^{th} eigenvector of ∇^2 evaluated on the t^{th} timeslice, sorted by eigenvalue. \square_t can also be written in terms of the eigenvectors

$$\square_t(\mathbf{x}, \mathbf{y}) = \sum_{k=1}^N v_{k,t}(\mathbf{x}) v_{k,t}^\dagger(\mathbf{y}) \quad (34)$$

\square projects into V_N , the subspace spanned by the N lowest eigenmodes, hence $\square^2 = \square$. Quark fields can be smeared by applying the distillation operator onto them. They inherit all symmetry properties of the unsmeared fields.

$$\chi^{(f)}(\mathbf{x}, t) \equiv \sum_{\mathbf{y}} \square_t(\mathbf{x}, \mathbf{y}) \psi^{(f)}(\mathbf{y}, t) \quad (35)$$

In essence the advantage of using smearing instead of the conventional smearing operator from which we started is the replacement of the gaussian shaped curve by a heaviside function. This enables one to calculate all-to-all propagators by inverting only a small number of modes.

3.2 Smearing behaviour of distillation

Expanding a local meson state $|\psi\rangle$ in a basis of eigenvectors of the lattice laplacian the state can be written as

$$\begin{aligned} |\psi\rangle &= \sum_k^M |v_k\rangle \langle v_k | \psi \rangle \\ \psi(\mathbf{x}) &= \sum_k^M \langle \mathbf{x} | v_k \rangle \langle v_k | \psi \rangle \end{aligned} \quad (36)$$

If we restrict the eigenmodes to some number N , this equation becomes the distillation operator (34). Hence the more eigenmodes we remove, the larger the width of the wave $\psi(\mathbf{x})$ becomes.

The same is true for distillation. To compute physical properties of mesonic states they have to be implemented on a lattice which lattice spacing corresponds to the size of a meson. Using local meson creation operators like (16) are not adequate because they only create a meson on a fixed lattice points. Hence it is crucial to apply smearing to the states. Similar to Gaussian smearing, the distilled quark is of Gaussian shape. If too many eigenmodes are removed the error of the results grow.

3.3 Distilled meson two-point correlation functions

Meson two-point correlation functions of distilled fields can be constructed starting from the definition (17) of the correlation function:

$$\begin{aligned} C(t_2 - t_1) &= \langle \Omega | \mathcal{O}^\dagger(t_2) \mathcal{O}(t_1) | \Omega \rangle \\ &= \pm \langle \Omega | \bar{\psi}^{(f_1)}(\mathbf{x}_1, t_2) \square_{t_2}(\mathbf{x}_1, \mathbf{y}_1) \Gamma^A \square_{t_2}(\mathbf{y}_1, \mathbf{x}_2) \psi^{(f_1)}(\mathbf{x}_2, t_2) \\ &\quad \times \bar{\psi}^{(f_2)}(\mathbf{x}_3, t_1) \square_{t_1}(\mathbf{x}_3, \mathbf{y}_2) \Gamma^B \square_{t_1}(\mathbf{y}_2, \mathbf{x}_4) \psi^{(f_2)}(\mathbf{x}_4, t_1) | \Omega \rangle \end{aligned} \quad (37)$$

Executing the same steps as in (25) yields

$$C(t_2 - t_1) = \langle Tr[\Phi^B(t_2) \tau^{(f_1)}(t_2, t_1) \Phi^A(t_1) \tau^{(f_2)}(t_1, t_2)] \rangle \quad (38)$$

In the last line the following definitions were used

$$\begin{aligned}\Phi_{AB}^A(t) &\equiv V_t^\dagger \Gamma_{AB}^A(t) V_t \\ \tau_{AB}(t_2, t_1) &\equiv V_{t_2}^\dagger (D^{-1})_{AB}(t_2, t_1) V_{t_1}\end{aligned}\tag{39}$$

$\Phi^A(t)$ is called the distilled gamma matrix and $\tau(t_2, t_1)$ the perambulator. The latter contains information about the quark propagator from every spatial point on timeslice t to every spatial point on timeslice t' .

Similar to V_t , $\tau_{AB}(t_2, t_1)$ is a complex $N \times N$ matrix where N is the number of eigenvectors used. The complete perambulator holds therefore $T^2 \times 4^2 \times N^2$ complex numbers. Similarly $\Phi_{AB}^A(t)$ is also a $N \times N$ matrix and the complete distilled gamma matrix has $T \times 4^2 \times N^2$ complex entries. Both matrices can be calculated independently from each other.

3.4 Computation of the perambulator

The propagator $(D^{-1(f)})_{AB}^{ab}(x; y)$ is defined by the following equation [1]

$$\sum_y (D^{(f)})_{AB}^{ab}(x; y) (D^{-1(f)})_{BC}^{bc}(y; z) = \delta_{ac} \delta_{AC} \delta(x, z)\tag{40}$$

To calculate the perambulator one computes solutions to the following linear equation, in the following text named "inversions",

$$\begin{aligned}\sum_x (D^{(f)})_{AB}^{ab}(x; y) \psi_B^{(f)b}(y) &= \xi_A^a(x) \\ \psi_B^{(f)b}(y) &= \sum_x (D^{-1(f)})_{BA}^{ba}(y, x) \xi_A^a(x)\end{aligned}\tag{41}$$

where $\xi(x)$ is the so called source term, also a fermionic field. Recall the definition of the perambulator (39), writing it explicitly will enable us to identify the inversion in the last equation [6]

$$\begin{aligned}\tau_{AB}(t_2, t_1) &\equiv V_{t_2}^\dagger (D^{-1})_{AB}(t_2, t_1) V_{t_1} \\ &= \sum_{k=1, k'=1}^N \sum_{x, y} v_{k, t_2}^{\dagger a}(\mathbf{x}) (D^{-1(f)})_{AB}^{ab}(\mathbf{x}, t_2; \mathbf{y}, t_1) v_{k', t_1}^b(\mathbf{y}) \\ &= \sum_{k=1, k'=1}^N \sum_{\mathbf{x}, \mathbf{y}, x_0, y_0} v_{k, t_2}^{\dagger a}(\mathbf{x}) \delta_{AA'} \delta_{t_2 x_0} (D^{-1(f)})_{A'B'}^{ab}(\mathbf{x}, x_0; \mathbf{y}, y_0) v_{k', t_1}^b(\mathbf{y}) \delta_{BB'} \delta_{t_1 y_0}\end{aligned}\tag{42}$$

The inversion (41) can now be identified

$$\psi_{A; B, t', k'}^{(f)a}(\mathbf{x}, x_0) = (D^{-1(f)})_{A'B'}^{ab}(\mathbf{x}, x_0; \mathbf{y}, y_0) v_{k', t'}^b(\mathbf{y}) \delta_{BB'} \delta_{t' y_0}\tag{43}$$

The indices B, t', k' express that $\psi_{A; B, t', k}^{(f)a}(\mathbf{x}, t)$ is defined on time slice t' and spin index B for the k'^{th} eigenvector.

The source terms $\xi(x)$ can also be identified:

$$\xi_{B; B', t', k'}^a(\mathbf{y}, y_0) = v_{k', t'}^b(\mathbf{y}) \delta_{BB'} \delta_{t' y_0}\tag{44}$$

The source terms are fields of the necessary size $L^3 \times 4 \times 3$ but have non-zero entries only at one specific spin index and timeslice.

Finally, equation (42) becomes:

$$\tau_{A'B'}^{(f)}(t_2, t_1) = \sum_{k=1, k'=1}^N \sum_{\mathbf{x}, x_0; \mathbf{y}, y_0} \xi_{A;A', t_2, k}^{\dagger a}(\mathbf{x}, x_0) \psi_{A;B', t_1, k'}^{(f)a}(\mathbf{y}, y_0) \quad (45)$$

To compute the complete perambulator one needs to compute $T \times 4 \times N$ inversions for all values of B, t', k and then multiply these with the hermitian conjugate of the sources as shown in equation (42). The eigenvectors were computed using a program provided inside the contraction code written by members of our work group. The source terms were calculated using code written by a previous bachelor student [6] and then submitted to the program `tmLQCD` [4] which calculates the inversions. Details about the implementation can be found in section 4.

4 Implementation

4.1 Overview

The computation of the correlation function on one gauge configuration can be broken down into the following steps

1. computation of N eigenvectors
2. generation of $T \times 4 \times N$ sources
3. computation of an inversion for every source
4. calculation of the perambulator and distilled gamma matrices
5. computation of the correlation function

This work builds on the contraction code written by members of our group and the aforementioned `tmLQCD` package. For documentation about steps 1 through 3 please see [6].

4.2 Programs

The following programs written in C++11 were added to the existing contraction code in `.../distillation/`. Every module consists of a `main.cpp`, a `module.h` and a `module.cpp` file. The documentation of each function can be found in the corresponding `.h` file.

- `perambulator/`: Calculates the perambulator using the sources and inverted sources.
- `distilled_gamma/`: Computes the distilled gamma matrix given the calculated eigenvectors.
- `correlator_trace/`: Computes the correlator for a given perambulator and distilled gamma matrix.

In addition to the above a `MultiVector` class has been written which can store a matrix of arbitrary dimension. Such a matrix can then be written to the disk. The definition of this class can be found in `helper/multivector.hpp`. It is used to store the perambulator, distilled gamma matrix and correlator trace.

For a more technical documentation see the provided `README` files and comments inside the source code.

4.2.1 Computation of the perambulators

This program computes the perambulator for all sources and inverted sources in two directories. The sources and the inverted sources *have to be* in the format

```
source.CONF-ID.time##.vec##.spin#
source.CONF-ID.time##.vec##.spin#.CONF-ID.00.inverted
```

respectively. Here `#` stands for a digit and `CONF-ID` is usually a 4-digit number. The program will read in all sources and inverted sources for one pair (k, k') into memory at once. This was done to reduce the times source terms were read from disc which proved to be a major performance factor. Hence running the program uses, for the gauge configurations used, about 48GB of RAM.

The program can be started by calling

```
./perambulator path-to-sources path-to-inverted-sources conf_id
                path-to-target-dir num_vec T L
```

where `num_vec` is the total number of eigenvectors N , T is the time dimension and L the spacial dimension of the lattice. Both `path-to-sources` and `path-to-inverted-sources` are paths to the directory where the sources and inverted sources live. The perambulator will be saved to the directory given by `path-to-target-dir` in the format

```
perambulator.CONF-ID.num_vec##.time##
```

using the `MultiVector` storage type mentioned earlier.

4.2.2 Computation of the distilled gamma matrix

This program computes the distilled gamma matrix for a given eigenvector. The gamma matrix Γ can be changed inside the source code. The distilled gamma matrix will be saved in the format

```
gamma.CONF-ID.num_vec##.time##
```

again using the `MultiVector` storage type.

The program can be started by calling

```
./gamma path-to-ev conf_id path-to-target-dir num-vec T L
```

`path-to-ev` is the path to the file which holds the eigenvectors.

4.2.3 Computation of the correlation function

To calculate the correlation function call

```
./trace path-to-gamma-matrix path-to-perambulator conf_id
      path-to-target-dir num_vec T
```

Here `path-to-gamma-matrix` and `path-to-perambulator` are the paths to the files holding the distilled gamma matrix and perambulator calculated earlier. The correlator will be saved in the format

```
trace.CONF-ID.num_vec##.time##
```

This file will contain all T^2 elements of the correlation function. To read the trace and calculate the mean values for every Δt run

```
./trace -r path-to-trace T
```

This will print all values in the format

$$\Delta t \text{ real}(C) \text{ imag}(C)$$

where C is the correlation function. The output of this operation is the basis for the results in section 5.

4.2.4 Python control script

In addition to the modules already mentioned a python script to control the simulation was written. It can find all files necessary for the simulation and can set up slurm job scripts (which are necessary on the *FUCHS* super computer) automatically. The script can be found inside the folder `.../distillation/scripts/` alongside its documentation. To start the script run

```
./run.py
```

The script will walk you through the setup process. It is written in python version 3.6.

5 Results

5.1 Lattice setup

Gauge configurations in this work were obtained from the ensemble A40.24 which has been generated using $N_f = 2 + 1 + 1$ quark flavors. Details can be looked up in [2]. The number of configurations was kept comparatively small since this work is only a first test of distillation.

# used configurations	β	κ	$a\mu_I$	$a\mu_\sigma$	$a\mu_\delta$	$(L/a)^3 \times T$
11	3.9	0.160856	0.0040	0.150	0.190	$24^3 \times 48$

Table 2: Parameters of gauge configurations used

5.2 Meson masses

To investigate the correctness and efficiency of the method of distillation described in this thesis computations of charmonium correlation functions were performed. These allow to test different configurations of eigenvectors in relatively short times compared to the use of light doublet states. Beside the number of gauge configurations the number of eigenvectors can be set arbitrarily. In this section I will present the results for 1, 2, 5 and 10 eigenvectors on the 11 gauge configurations mentioned in the previous section.

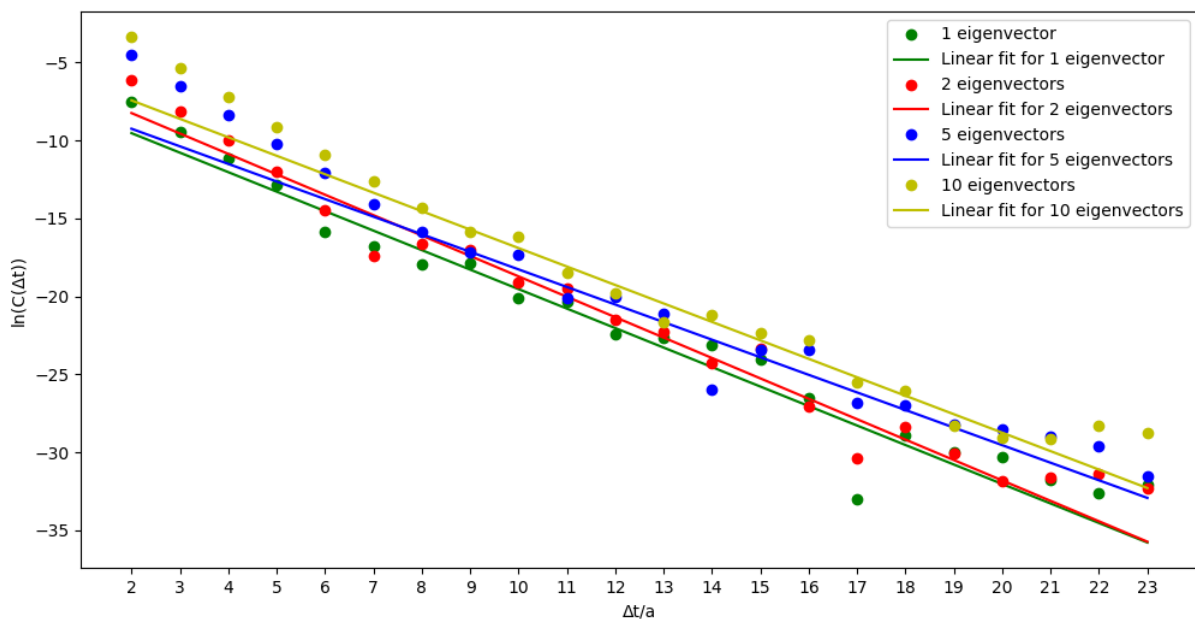


Figure 1: Combined results for 1, 2, 5 and 10 eigenvectors

In all computations the following creation operator was used:

$$\mathcal{O}(t) = \bar{\chi}^{(c)}(t)\gamma_5\chi^{(c)}(t) \quad (46)$$

Therefore the resulting meson has quantum numbers $0(0^-)$ [5] which therefore corresponds to a η_c meson with a mass of $2983.4 \pm 0.5\text{MeV}$ [8]. This was achieved by using for both propagators ($D^{-1(f)}$) the same flavor f . This approach reduced the amount of inversions that had to be calculated by a factor of two. For the same reason a charmonium state was chosen in contrast

to e.g. the calculation of a pion mass. Inversions for particles with higher masses converge significantly faster.

To compute the mass of the charmonium state the mean value of all configurations for one value of Δt were computed and a simple linear function was fitted to $\ln(C(\Delta t))$. The results for 1, 2, 5 and 10 eigenvectors can be seen in figure 1. One can see the similar shapes of all four results. Because the exponential nature of the correlation function holds for $\Delta t \rightarrow \infty$ only a few points were chosen to be fitted. In figure 2 one can see the four results side by side. The points which were used to fit the linear function are colored differently.

The masses of these four simulations are shown in table 3, the errors were calculated using the *Jackknife* [11] method.

Number of eigenvectors	Mass (MeV)
1	3082 ± 255
2	3227 ± 215
5	2780 ± 91
10	2919 ± 88

Table 3: Calculated masses for the charmonium state

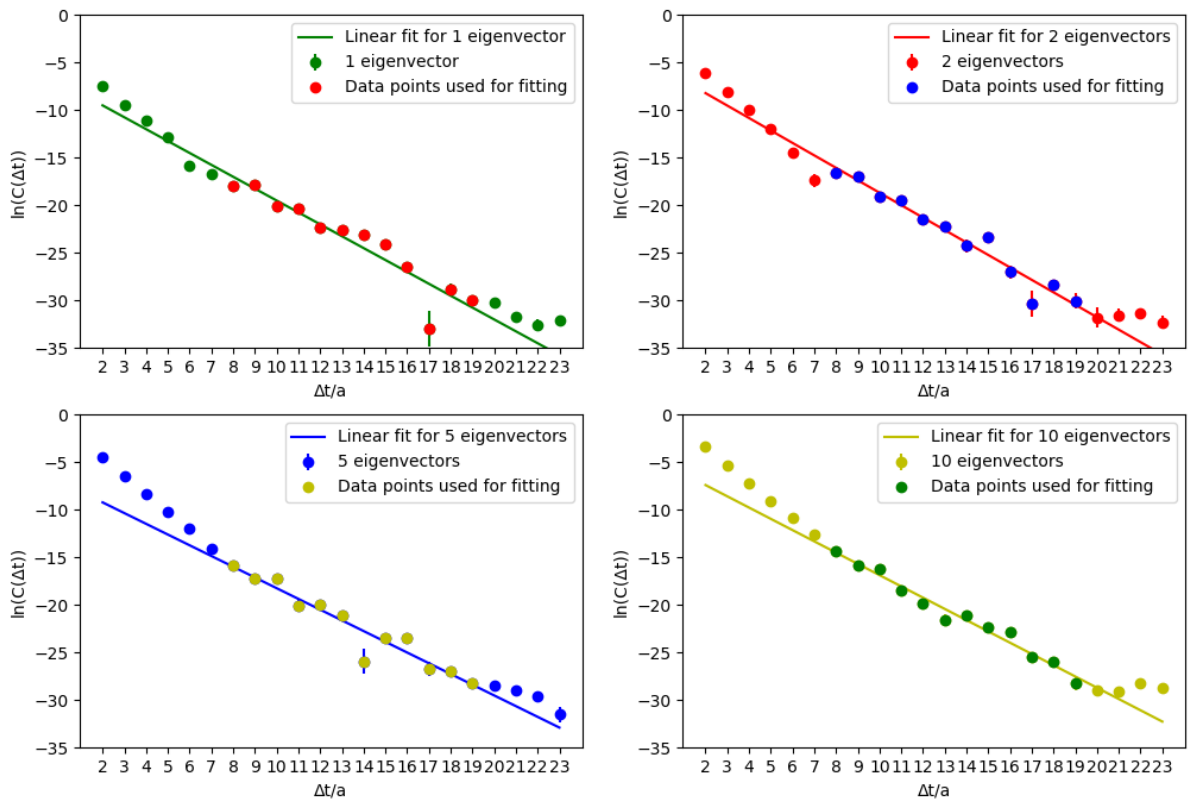


Figure 2: Logarithmic results for 1, 2, 5 and 10 eigenvectors with error bars. The data points used for fitting are colored differently.

Looking at figure 1 one can see that a small number of eigenvectors corresponds to a small value of $C(t)$. Also one can see that computations with a higher number of eigenvectors the asymptotic slope is reached earlier.

6 Discussion

6.1 Complexity of the simulation depending on the number of eigenvectors

Throughout this section I will assume a lattice of size of $24^3 \times 48$.

The complexity of the simulation increases linearly with the number of configurations. When changing the number of eigenvectors the simulation will be affected in different steps in a different way:

- Naturally the time to calculate all eigenvectors depends **linearly** on the number of eigenvectors.
- The number of source and inverted source terms depend **linearly** on the number of eigenvectors as well. Therefore the same holds true for the time to calculate these.
- Computation times of the distilled gamma matrix increases **quadratically** with the number of eigenvectors.
- The time to calculate the perambulator depends quadratically on the number of source terms used and therefore also **quadratically** on the number of eigenvectors. The time of calculations depends here especially on the reading process of the source terms. This proved to be a major factor influencing the performance.
- As the last step the calculation of the correlation function depends on the number of eigenvectors **to the fourth**.

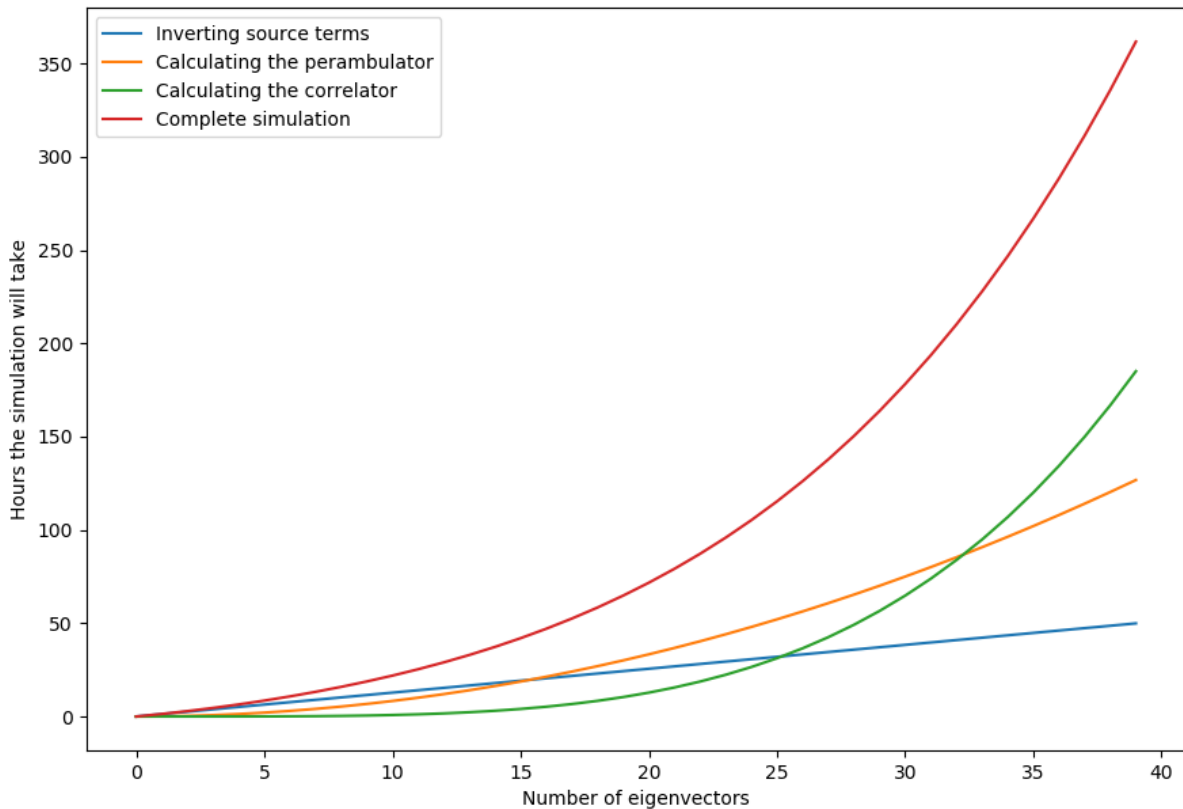


Figure 3: Distribution of the time the simulation will take

The inversion of the source terms took for the number of eigenvectors shown in section 5 the longest, followed by the computation of the perambulator. Calculating time for the eigenvectors, source terms and gamma matrix can be safely neglected in comparison. The correlator (with its N^4 dependence) on the other hand can also be neglected for small ($N < 5$) number of eigenvectors but starts to play a major role when increasing the number of eigenvectors.

Inverting a single source term takes, when calculating the mass of a charmonium state, about 20 minutes per thread on the *FUCHS* super computer. Calculating the perambulator for one eigenvector takes about 5 minutes. The last step, computing the correlator, needs for a single eigenvector circa 0.3 seconds. For the perambulator and correlator the time was determined from the time each step runs for when using 5 eigenvectors.

In figure 3 a plot of the time each of these steps will run for with respect to the number of eigenvectors can be seen. The curves were interpolated by the time measured when calculating 1, 2, 5 and 10 eigenvectors.

This is of course a rough estimate, the actual time depends on a series of factors, e.g. differences between different computation nodes. It is also important to keep disc space constraints (ROM) in mind. The following table shows the space the files for each step need. One can see that the source terms and their corresponding inverted counterparts will start to use a lot of disc space when using a higher number of eigenvectors. When computing the correlator with $N = 10$ on 11 configurations, all source terms combined used about 2.6TB of disc space.

Step	Approximate space needed
eigenvectors	$6\text{MB} \times N$
(inverted) source terms	$61\text{MB} \times T \times 4 \times N$
perambulator	$0.6\text{MB} \times N^2$
gamma matrix	$12\text{KB} \times N^2$
correlator	37KB

Table 4: Disc space each step needs

6.2 Outlook

This work represents a first test of distillation by Marc Wagner's work group, therefore the number of eigenvectors and gauge configurations was kept small.

The results show that calculating meson masses using distillation is feasible. The particle in question is a light η_c charmonium with a mass of $2983.4 \pm 0.5\text{MeV}$ [8]. Even using only 11 gauge configurations a value close to that in the literature was observed. The results also show that a greater number of eigenvectors has a notable effect on the accuracy of the simulation. It appears preferably to use at least ten eigenvectors to reduce the error of the results. An increase of configuration will also play a large role in improving the simulation. Further tests will be needed to find a good balance between the number of eigenvectors and configurations.

Before attempting a computation of greater scale, a few improvements to the method can and should be made: Especially to reduce the space and time needed the source terms should be written into a single file. It probably has to be split again to be used by the inverter, but the computation of the perambulator will be sped up significantly if the program only needs to read one file into memory. Another step would be to utilize parallelism when computing the perambulator, eigenvectors and correlator.

7 References

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Selbstständigkeitserklärung

Erklärung nach § 30, (12) Ordnung für den Bachelor- und den Masterstudiengang

Hiermit erkläre ich, dass ich die Arbeit selbstständig und ohne Benutzung anderer als der angegebenen Quellen und Hilfsmittel verfasst habe. Alle Stellen der Arbeit, die wörtlich oder sinngemäß aus Veröffentlichungen oder aus anderen fremden Texten entnommen wurden, sind von mir als solche kenntlich gemacht worden. Ferner erkläre ich, dass die Arbeit nicht - auch nicht auszugsweise - für eine andere Prüfung verwendet wurde.

Ort, Datum

Lars Gröber