# Bachelor Thesis

# *Computation of meson correlation functions using distillation: Generation of propagators*

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# Abstract

In this work quark propagators are computed via distillation for mass degenerate up and down quarks using Wilson twisted mass fermions. The computations are performed on a set of 11 gauge configurations. The gauge configurations correspond to $N_f = 2 + 1 + 1$ mass degenerate up and down sea and valence quarks plus mass split strange and charm sea quarks. The computations are performed on a lattice of size $(L/a = 24)^3 \times (T/a = 48)$ using distillation with 5 eigenvectors of the gauge covariant lattice Laplacian.


# Contents

# 1. Introduction

It appears to be an impelling need of humanity trying to understand the fundamental principles and laws of nature and to investigate the elementary building blocks of matter which are called particles. The physicists current answer to these questions is the so called *Standard Model* that includes all particles that are supposed to be elementary according to the current state of science. The Standard Model also describes the interactions of these elementary particles via three of the four fundamental forces namely the electromagnetic force, the weak force and the strong force.

This work will focus on particles interacting via the strong force that is described by a mathematical framework called *quantum chromodynamics* (QCD). The elementary particles interacting via the strong force are called quarks and they interact with each other via the exchange of so called gauge bosons - the gluons. Quarks appear in six different flavours and are characterised by a set of properties like mass and the so called quantum numbers, e.g. electric charge, spin, total angular momentum, color charge, etc. Quarks are fermions - all of them have spin 1/2. There are also antiquarks that differ from their non-anti counterparts in opposite signs of all charge-like quantum numbers.

Gluons are the force carriers of the strong force. As different particles with different properties the eight gluons are described by a different set of quantum numbers. First of all, they are massless and as a boson the gluon has an integer spin taking the value 1. The most interesting property of the gluons is that they carry a color charge. Likewise, the electric charge is the field-generating quantity in electrodynamics, the color charge is the source of the strong force. Having a color charge means for a gluon that it can interact with other gluons.

Particles composed of quarks and antiquarks are called hadrons. One distinguishes between hadrons composed of a quark-antiquark pair - the mesons and bound states of three valence quarks - the baryons. But there are so called exotic hadrons as well. The properties of hadrons arise from the quantum numbers of their constituents. These properties are measurable quantities that can be obtained in experiments and it is essential for a theory like QCD to reproduce the measured results to a certain precision. Unfortunately, in QCD physical observables are very difficult to obtain by analytical computations due to the high complexity of the mathematical framework. A way to deal with this problem, that gained popularity due to the increasing computational power of modern computers, is the numerical treatment of QCD.

QCD can be treated effectively on computers if it is reformulated on a lattice of discrete points in spacetime. This approach is known as *lattice QCD*. In this thesis lattice QCD is used to calculate quark propagators that are needed for the computation of meson masses. Meson masses can be obtained from a so called temporal correlation functions or correlators that are vacuum expectation values of hadron creation operators. A correlation function can be evaluated numerically and the meson mass can be extracted from a fit of the correlator that exponentially decreases in time.

Apart the constraint that the hadron creation operators have to create the right quantum numbers of the meson under investigation, there is some degree of freedom in their construction. This ambiguity is utilized by a method called *distillation*. Distillation is a way of constructing hadron creation operators using eigenvectors of the lattice Laplacian. This method provides the possibility to compute all-to-all quark propagators not only in principle but also in practice. Further distillation is suitable for observing ground states of hadronic spectra with small statistical errors.

The numerical computation of all-to-all quark propagators using the method of distillation is the subject of this thesis.

# 2. Theoretical basics

## 2.1. Conventions

Physical units are chosen in a way that velocities are measured in units of the speed of light $c$ and actions are measured in units of the reduced Planck constant $\hbar$, i.e., **natural units** are used in this work:

$$c = \hbar = 1.$$

On the lattice **energies** are measured **in units of the inverse lattice spacing** $a^{-1}$.

If there are equations with an index appearing twice and no explicit summation is written down, the **Einstein notation** has been used, i.e., there is an implicit summation over these indices.

The **euclidean formulation of QCD** is used by substituting the real time $x_0$ by the imaginary time $x_0 = -ix_4$. Consequently the Minkowski metric tensor is replaced by the unit matrix:

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The euclidean Dirac matrices are defined to possess the following properties:

- $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$
- $\{\gamma_5, \gamma_\mu\} = 0$ with $\gamma_5 \equiv \gamma_1\gamma_2\gamma_3\gamma_4$
- $\gamma_\mu^2 = \gamma_5^2 = 1$ for $\mu = 1, 2, 3, 4$

## 2.2. QCD

QCD is a quantum field theory (QFT). In such a theory particles are treated as discrete excitations of fields. A field is a function that maps a mathematical object, e.g. a scalar, vector, spinor or tensor, etc. to every point $x$ in spacetime. All physical information of QCD is encoded in its action [1]:

$$S_{\mathrm{QCD}}[\psi, \bar{\psi}, A] = \int d^4x \Big( \underbrace{\sum_{f=1}^{N_f} \bar{\psi}^{(f)}(x)(\gamma_\mu D_\mu + m^{(f)})\psi^{(f)}(x)}_{\text{fermionic part}} + \underbrace{\frac{1}{4} \sum_{a=1}^{8} F^a_{\mu\nu}(x) F^a_{\mu\nu}(x)}_{\text{gauge part}} \Big). \tag{2.1}$$

QCD is a $SU(3)$ gauge theory, i.e., the action (2.1) is invariant under local $SU(3)$ transformations. The $SU(3)$ symmetry defines QCD and gives rise to its distinct properties.

Further the QCD action is invariant under local $U(1)$ transformations. The approximate flavour symmetry of the theory is broken because quarks of different flavours have different masses in nature. QCD has some discrete symmetries as well, like parity and charge conjugation.

The fermionic part of the action (2.1) contains information about the dynamics of QCD's fermionic degrees of freedom, i.e., the quarks and it determines the coupling of the quarks to the gluons. The gauge part describes the dynamics and self interactions of the gluons.

$D_\mu$ denotes the gauge-covariant derivative:

$$D_\mu = \partial_\mu - igA_\mu(x) \;=\; \partial_\mu - ig\sum_{a=1}^{8} T^a A_\mu^a(x). \tag{2.2}$$

To be gauge-covariant means that $D_\mu$ does not change its form under local $SU(3)$ transformations. The constant $g$ is the bare coupling of the theory. $T^a$ are $SU(3)$ generators, i.e, they are the elements of the Lie algebra of $SU(3)$.

The field strength tensor $F_{\mu\nu}(x) = T^a F_{\mu\nu}^a(x)$ is defined by the following commutator:

$$F_{\mu\nu} = -\frac{i}{g}\left[D_\mu, D_\nu\right] \tag{2.3}$$

$$= \partial_\mu A_\nu - \partial_\nu A_\mu - ig\left[A_\mu, A_\nu\right] \tag{2.4}$$

$$= \partial_\mu A_\nu - \partial_\nu A_\mu - ig\; A_\mu^a A_\nu^b \left[T^a, T^b\right] \tag{2.5}$$

$$= \partial_\mu A_\nu - \partial_\nu A_\mu + g\; f^{abc} A_\mu^a A_\nu^b T^c \tag{2.6}$$

$$= T^c \underbrace{\left(\partial_\mu A_\nu^c - \partial_\nu A_\mu^c + g\; f^{abc} A_\mu^a A_\nu^b\right)}_{F_{\mu\nu}^c}. \tag{2.7}$$

In the step from (2.5) to (2.6) the Lie algebra of $SU(3)$ $\left[T^a, T^b\right] = if^{abc}T^c$ with the structure constants $f^{abc}$ has been used.

The quark fields $\psi$ and $\bar{\psi} = \psi^\dagger\gamma_4$ internal degrees of freedom are listed in Table 1. Single components of the quark fields are notated as $\psi_A^{(f),c}(x)$ respectively $\bar{\psi}_A^{(f),c}(x)$.

| degree of freedom | index | number of components |
|---|---|---|
| spin | $A$ | 4 |
| color | $c$ | 3 |
| flavour | $f$ | $N_f$ |

Table 1: Structure of quark fields

The gluon fields $A_\mu(x)$ appear with eight color degrees of freedom that mathematically correspond to the fact that the gluons transform under the adjoint representation of $SU(3)$.

The fermionic part of the action (2.1) gives rise to quark-gluon interactions:

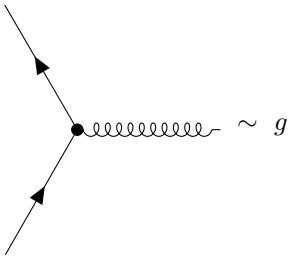


Figure 1: Quark-gluon vertex [2]

Because the gluon field strength tensor $F_{\mu\nu}$ is quadratic in $A_\mu$ and appears quadratic in $\mathcal{L}_{QCD}$ there are gluon self-interactions up to order $g^2$:


Figure 2: Three-gluon vertex and Four-gluon vertex

## 2.3. Lattice QCD

In order to do numerical QCD calculations continuous spacetime is replaced by a 4 dimensional lattice of discrete spacetime points. The lattice is defined by a set of points:

$$\Lambda_4 = \{n = (\mathbf{n}, n_4) \mid 0 \leq n_\mu \leq L_\mu\}\,, \qquad \mu = 1, 2, 3, 4. \tag{2.8}$$

The implementation on a computer necessitates the use of a finite lattice. Usually the spatial dimensions are chosen to be $L_1 = L_2 = L_3 \equiv L$. The introduction of a finite lattice breaks the translational invariance of the theory. Hence momentum conservation would be violated. The introduction of periodic boundary conditions fixes that issue:

$$n + L_\mu \hat{\mu} = n\,, \qquad \hat{\mu}\text{: unit vector in direction } \mu. \tag{2.9}$$

The introduction of a finite lattice with periodic boundaries furthermore implies the discretization of momenta.

QCD has to be reformulated after introducing the lattice. The continuum action (2.1) is transferred into the lattice action:

$$S_{\mathrm{QCD}}[\psi,\bar{\psi},A] \quad \rightarrow \quad S_{\mathrm{Lattice\ QCD}}[\psi,\bar{\psi},U] \equiv S[\psi,\bar{\psi},U]. \tag{2.10}$$

The lattice action should preserve as many symmetries of the continuum action as possible, especially the $SU(3)$ gauge symmetry. To ensure gauge invariance of the fermionic part of the action the continuum gauge field $A_\mu(x)$ has to be replaced by a new type of field $U_\mu(n)$ called link variable. While $A_\mu$ is an element of the Lie algebra of $SU(3)$ the link variable $U_\mu$ is an element of $SU(3)$ itself:

$$U_\mu(n) = e^{-igA_\mu(n)}. \tag{2.11}$$

The lattice action is constrained to become the continuum action in the continuum limit, i.e., for the lattice spacing $a$ going to zero. A possible realization of a lattice gauge action that obeys this condition is the Wilson gauge action [1]:

$$S_U[U] = \beta \sum_{n\in\Lambda_4} \sum_{\mu<\nu} \mathrm{Re\,tr}\left[1 - U_{\mu\nu}(n)\right]. \tag{2.12}$$

$\beta \equiv 6/g^2$ with the bare coupling constant $g$ as it appears in (2.2). The so called plaquette $U_{\mu\nu}(n)$ is the simplest non-trivial closed loop of link variables on the lattice:

$$U_{\mu\nu}(n) = U_\mu(n)U_\nu(n+\hat{\mu})U_\mu^\dagger(n+\hat{\nu})U_\nu^\dagger(n). \tag{2.13}$$

Any closed loop of link variables like the plaquette is gauge invariant in general. $U_{\mu\nu}(n)$ can be visualized by the following diagram:

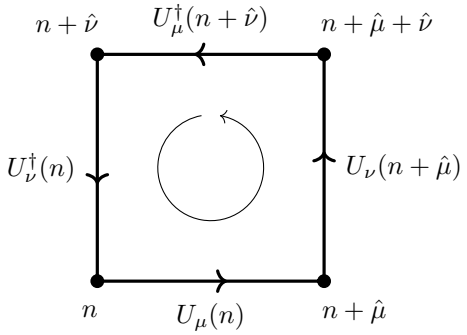


Figure 3: The plaquette $U_{\mu\nu}(n)$

The summation in (2.12) is equivalent to a sum over all plaquettes that are located on the lattice.

The choice of the gauge action is not unique, hence other valid realisations of $S_U$ can be implemented on the lattice as well, e.g. [3].

Discretizing the fermion action is accompanied by difficulties. The first obvious guess for the fermion action that is gauge invariant and has the correct continuum limit is:

$$S_F[\psi,\bar{\psi},U] = \sum_{f=1}^{N_f}\sum_{n\in\Lambda_4}\bar{\psi}^{(f)}(n)\Big(\sum_{\mu=1}^{4}\frac{U_\mu(n)\;\psi^{(f)}(n+\hat{\mu}) - U_\mu^\dagger(n-\hat{\mu})\;\psi^{(f)}(n-\hat{\mu})}{2} - m^{(f)}\psi^{(f)}(n)\Big)$$

$$= \sum_{f=1}^{N_f}\sum_{n,m\in\Lambda_4}\bar{\psi}_A^{(f),a}(n)\;(D^{(f)})_{AB}^{ab}(n;m)\;\psi_B^{(f),b}(m). \tag{2.14}$$

In the last line the lattice Dirac operator for some quark flavor $f$ is introduced:

$$(D^{(f)})_{AB}^{ab}(n;m) = (\gamma_\mu)_{AB}\sum_{\mu=1}^{4}\frac{(U_\mu)^{ab}(n)\;\delta_{n+\hat{\mu},m} - (U_\mu^\dagger)^{ab}(n-\hat{\mu})\;\delta_{n-\hat{\mu},m}}{2} + m^{(f)}\delta_{A,B}\delta_{a,b}\delta_{n,m}. \tag{2.15}$$

Unfortunately the propagator defined as the inverse of (2.15) creates unphysical quark degrees of freedom that do not vanish in the continuum limit $a \to 0$. These degrees of freedom are pure lattice artifacts, hence the obvious guess for the fermion action is not a valid guess. This problem is referred to as *fermion doubling* [1].

There can be found fermionic lattice actions of the form (2.14) using another choice of the lattice Dirac operator preventing fermion doubling. One approach is to add an additional mass term in the Dirac operator at the price of breaking chiral symmetry that continuum QCD possesses for vanishing quark masses. The corresponding fermions are called *Wilson fermions* [1].

The fermion action that is used for the numerical calculations in this thesis is the *Wilson twisted mass action* [4]. This approach is valid for mass degenerate quarks $m^{(u)} = m^{(d)} \equiv m$:

$$\begin{aligned} S_F[\chi,\bar{\chi},U] = \sum_{n\in\Lambda_4}\Big(&\bar{\chi}(n)(1+i2\kappa\mu_l\gamma_5\tau_3)\chi(n) \\ &- \kappa\sum_{\mu=1}^{4}\bar{\chi}(n)U_\mu(n,n+\hat{\mu})(1-\gamma_\mu)\chi(n+\hat{\mu}) \\ &- \kappa\sum_{\mu=1}^{4}\bar{\chi}(n)U_\mu^\dagger(n,n-\hat{\mu})(1+\gamma_\mu)\chi(n-\hat{\mu})\Big). \end{aligned} \tag{2.16}$$

$\tau_3$ denotes the third Pauli matrix acting in flavor space. The doublet $\chi \equiv (\chi^{(u)},\chi^{(d)})$ does not contain the physical quark fields. $\chi$ is related to the physical quark doublet $\psi = (\psi^{(u)},\psi^{(d)})$ via the transformation: $\psi = e^{i\omega\gamma_5\tau_3/2}\chi$ respectively $\bar{\psi} = \bar{\chi}e^{i\omega\gamma_5\tau_3/2}$. The parameters that are required as input for the computations are the twisted quark mass $\mu_l$ and the hopping parameter $\kappa$ that is defined as [4]:

$$\kappa = \frac{1}{8+2m}. \tag{2.17}$$

Combining the the gauge action and the fermion action yields the lattice action of QCD:

$$S[\chi,\bar{\chi},U] = S_F[\chi,\bar{\chi},U] + S_U[U]. \tag{2.18}$$

# 3. Meson correlation functions

Correlation functions of hadron creation and annihilation operators are the fundamental objects of hadron spectroscopy. Hadronic energy spectra can be directly extracted from correlation functions by observing their temporal decrease. In this section the focus is set on correlation functions of meson creation and annihilation operators.

## 3.1. Meson creation operators

Mesons typically are quark anti-quark states. A meson state is characterized by a set of quantum numbers:

- Total angular momentum: $J \in \mathbb{N}$ since all mesons are bosons
- Parity: $P = \pm 1$
- Charge conjugation (for identical flavours): $C = \pm 1$
- Flavor quantum numbers listed in table 2

| | | **Flavor quantum numbers** | | | | |
|---|---|---|---|---|---|---|
| **Flavor** | | Isospin-$z$: $I_3$ | Strangeness: $S$ | Charm: $C$ | Bottomness: $B'$ | Topness: $T$ |
| up | **u** | +1/2 | 0 | 0 | 0 | 0 |
| down | **d** | -1/2 | 0 | 0 | 0 | 0 |
| strange | **s** | 0 | -1 | 0 | 0 | 0 |
| charm | **c** | 0 | 0 | +1 | 0 | 0 |
| bottom | **b** | 0 | 0 | 0 | -1 | 0 |
| top | **t** | 0 | 0 | 0 | 0 | 1 |

Table 2: Flavor quantum numbers of quarks

Neglecting flavor quantum numbers a meson state can be denoted with the quantum numbers $I(J^P)$ [5]. $I$ denotes the total isospin. To observe a particular meson state a meson creation operator has to be constructed that has the quantum numbers of this meson.

Aside the constraint that the operator has to carry suitable quantum numbers there is some freedom in its construction. In principle one could use any operator as meson creation operator as long as it has the quantum numbers of the meson under investigation. The simplest local meson creation operators basically have the form of bilinear covariants:

$$O(n) = \bar{\psi}^{(f_1)}(n)\Gamma\psi^{(f_2)}(n), \qquad O^\dagger(n) = \pm\bar{\psi}^{(f_2)}(n)\Gamma\psi^{(f_1)}(n). \tag{3.1}$$

The quark fields have to be chosen in a way to provide the desired quark flavors $f_1$ and $f_2$. $\Gamma$ is a matrix in Dirac space - usually a combination of Dirac matrices that correspond to total angular momentum $J$ and parity $P$.

The overall sign of the hermitian conjugate $O^\dagger(n)$ depends on $\Gamma$ since $\gamma_4\Gamma^\dagger\gamma_4 = \pm\Gamma$. Table 3 lists different $\Gamma$'s and the corresponding values of $J$ and $P$.

| Transformation law | $J$ | $P$ | $\Gamma$ | Particles |
|---|---|---|---|---|
| Pseudoscalar | 0 | -1 | $\gamma_5$, $\gamma_4\gamma_5$ | $\pi^{\pm}$, $\pi^0$, $\eta_c$, ... |
| Scalar | 0 | +1 | 1, $\gamma_4$ | $a_0$, $K_0^*$, ... |
| Vector | 1 | -1 | $\gamma_i$, $\gamma_4\gamma_i$ | $\rho^{\pm}$, $\rho^0$, $K^*$, ... |
| Axial vector | 1 | +1 | $\gamma_i\gamma_5$ | $a_1$, ... |
| Tensor | 1 | +1 | $\gamma_i\gamma_j$ | $b_1$, .. |

Table 3: $\Gamma$-structure and corresponding quantum numbers [1]

Some examples of local meson creation operators are:

- $K_0^*$: $O_{K_0^*}(n) = \bar{s}(n)d(n)$
- Pion $\pi^-$: $O_{\pi^-}(n) = \bar{u}(n)\gamma_5 d(n)$
- $\rho$ meson $\rho^+$: $O_{\rho^+}(n) = \bar{d}(n)\gamma_i u(n)$ with $i = 1, 2, 3$.

Acting on the vacuum $|\Omega\rangle$ a local creation operator $O(n)$ with quantum numbers $I(J^P)$ creates a field excitation with these quantum numbers localized at position $n$. The corresponding state can be expanded in the energy eigenbasis:

$$O(n)\,|\Omega\rangle = \sum_{k=0}^{\infty} |k\rangle \underbrace{\langle k|\, O(n)\,|\Omega\rangle}_{a_k} = \sum_{k=0}^{\infty} a_k\,|k\rangle\,. \tag{3.2}$$

$|k\rangle \equiv |I(J^P); k\rangle$ denotes an energy eigenstate corresponding to quantum numbers $I(J^P)$. The absolute value of the coefficient $a_k$ gives information how much the energy eigenstate $|k\rangle$ contributes to the superposition.

For example [5], computing the energy of a pion corresponds to observing the ground state $|1(0^-); 0\rangle$. Higher energy eigenstates are many particle pion states like $|\pi + \pi + \pi\rangle$ and excitations of the pion like the $|\pi(1300)\rangle$.

In order to investigate the ground state $|0\rangle$ the freedom of choosing any suitable $O(n)$ can be exploited. Creation operators can be constructed from *smeared* quark fields [6] such that the overlap $\langle 0|\, O(n)\,|\Omega\rangle$ has a large magnitude compared to the overlaps $\langle k|\, O(n)\,|\Omega\rangle$ of higher states ($k > 0$). Distillation can be viewed as a smearing as well.

In order to calculate energy spectra or particle masses one works with momentum projected meson creation operators that are obtained by spatial Fourier transformation of the local operators:

$$\tilde{O}(\mathbf{p}, n_4) = \sum_{\mathbf{n}\in\Lambda_3} O(\mathbf{n}, n_4) e^{-i\mathbf{n}\cdot\mathbf{p}}, \tag{3.3}$$

where the summation over $\mathbf{n}$ takes place over all points inside the spatial part of the lattice $\Lambda_3$. Due to the restriction of the lattice to a finite volume the spatial components of the momentum are $p_i = 2\pi m_i / L_i$ for $i = 1, 2, 3$ and $m_i \in \mathbb{Z}$.

For measuring a meson mass the local creation operator with the desired quantum numbers is projected to momentum **0** by summing over all spatial lattice sides:

$$\begin{aligned}\tilde{O}(n_4) &\equiv \tilde{O}(\mathbf{0}, n_4) \\ &= \sum_{\mathbf{n}\in\Lambda_3} O(\mathbf{n}, n_4).\end{aligned} \tag{3.4}$$

## 3.2. Correlation functions of meson creation operators

Correlation functions of meson creation operators, also called correlators, are vacuum expectation values (VEV's) of these operators. On the lattice VEV's are defined by the Feynman path integral as well as in continuum:

$$\langle\Omega|\, O^\dagger(n)O(m)\,|\Omega\rangle = \frac{1}{Z}\int \mathcal{D}[\psi]\mathcal{D}[\bar{\psi}]\int \mathcal{D}[U]\; O^\dagger(n)O(m)\; e^{-S[\psi,\bar{\psi},U]}. \tag{3.5}$$

$Z$ denotes the partition function:

$$Z = \int \mathcal{D}[\psi]\mathcal{D}[\bar{\psi}]\int \mathcal{D}[U]\; e^{-S[\psi,\bar{\psi},U]}. \tag{3.6}$$

$S[\psi,\bar{\psi},U]$ is the lattice action (2.18). By introducing a finite lattice intrinsic difficulties of the path integral are resolved. Divergent factors in the integration measure become finite and the infinite dimensional integration is replaced by a high but finite dimensional integral:

$$\int \mathcal{D}[\psi]\mathcal{D}[\bar{\psi}]\int \mathcal{D}[U] \sim \prod_{n\in\Lambda_4}\int d\psi(n)\, d\bar{\psi}(n)\int dU(n). \tag{3.7}$$

In order to extract the mesonic energy spectrum one computes correlators of momentum projected meson creation operators. By rewriting the correlation function in its spectral representation one can gain insight how the spectrum can be extracted. The first step consists of inserting a complete 1 of energy eigenstates:

$$\begin{aligned}C(t_2-t_1) &\equiv \langle\Omega|\, \tilde{O}^\dagger(t_2)\tilde{O}(t_1)\,|\Omega\rangle\;, \qquad\qquad t_2 > t_1 \\ &= \sum_{k=0}^{\infty}\langle\Omega|\, \tilde{O}^\dagger(t_2)\,|k\rangle\,\langle k|\,\tilde{O}(t_1)\,|\Omega\rangle\,.\end{aligned} \tag{3.8}$$

Now one can use that $\tilde{O}(t_2)$ is a Heisenberg operator whose temporal evolution is determined by the Hamiltonian $H$:

$$= \sum_{k=0}^{\infty}\langle\Omega|\, e^{H(t_2-t_1)}\tilde{O}^\dagger(t_1)e^{-H(t_2-t_1)}\,|k\rangle\,\langle k|\,\tilde{O}(t_1)\,|\Omega\rangle\,. \tag{3.9}$$

The exponentials act on the vacuum state and the inserted energy eigenstates:

$$\langle\Omega|\, e^{H(t_2-t_1)} = \langle\Omega|\, e^{E_\Omega(t_2-t_1)} \qquad e^{-H(t_2-t_1)}\,|k\rangle = e^{-E'_k(t_2-t_1)}\,|k\rangle\,. \tag{3.10}$$

Continue from equation (3.9):

$$
\begin{aligned}
&= \sum_{k=0}^{\infty} \langle\Omega|\, \tilde{O}^\dagger(t_1)\, |k\rangle\, \langle k|\, \tilde{O}(t_1)\, |\Omega\rangle\, e^{-(E'_k - E_\Omega)(t_2-t_1)} \\
&= \sum_{k=0}^{\infty} (\langle k|\, \tilde{O}(t_1)\, |\Omega\rangle)^\dagger\, \langle k|\, \tilde{O}(t_1)\, |\Omega\rangle\, e^{-(E'_k - E_\Omega)(t_2-t_1)} \\
&= \sum_{k=0}^{\infty} \underbrace{\left|\, \langle k|\, \tilde{O}(t_1)\, |\Omega\rangle\, \right|^2}_{|a_k|^2} e^{-E_k(t_2-t_1)}. \qquad (3.11)
\end{aligned}
$$

$E_k = E'_k - E_\Omega$ is the energy of state $|k\rangle$ measured relative to the infinite energy of the vacuum $E_\Omega$. $E_k$ is given by the relativistic energy momentum relation:

$$E_k = \sqrt{m_k^2 + \mathbf{p}^2}. \qquad (3.12)$$

Using meson creation operators projected to momentum $\mathbf{0}$ yields $E_k = m_k$. For large temporal separations $\Delta t = (t_2 - t_1)$ the sum (3.11) is dominated by the ground state since the other terms vanish quicker due to $m_k \gg m_0$ for $k > 0$:

$$\lim_{\Delta t \to \infty} C(t_2 - t_1) = |a_0|^2\, e^{-E_0(t_2-t_1)}. \qquad (3.13)$$

A large overlap $a_0 = \langle 0|\, \tilde{O}(t_1)\, |\Omega\rangle$ causes faster convergence of (3.11) to the ground state. Hence a smaller lattice can be used, i.e., computation time is saved by using creation operators of smeared quark fields. After computing the temporal progression of the correlator the energy or mass of the ground state can be extracted by an exponential fit of $C(t_2 - t_1)$.

The numerical computation can be done using the correlators definition via the path integral (3.5). The corresponding integration over the Grassmann-valued fermion fields can be performed by hand:

$$
\begin{aligned}
C(t_2 - t_1) &\equiv C(n_4 - m_4) \qquad (3.14) \\
&= \langle\Omega|\, \tilde{O}^\dagger(n_4) \tilde{O}(m_4)\, |\Omega\rangle \\
&= \pm \sum_{\mathbf{n},\mathbf{m} \in \Lambda_3} \langle\Omega|\, \bar{\psi}^{(f_2)}(\mathbf{n}, n_4) \Gamma \psi^{(f_1)}(\mathbf{n}, n_4)\; \bar{\psi}^{(f_1)}(\mathbf{m}, m_4) \Gamma \psi^{(f_2)}(\mathbf{m}, m_4)\, |\Omega\rangle\,.
\end{aligned}
$$

The $\pm$ sign arises from the hermitian adjoint meson creation operator (3.1).

$$
\begin{aligned}
&= \pm \sum_{\mathbf{n},\mathbf{m}} \langle\Omega|\, \bar{\psi}_A^{(f_2),a}(\mathbf{n}, n_4) \Gamma_{AB} \psi_B^{(f_1),a}(\mathbf{n}, n_4)\; \bar{\psi}_C^{(f_1),b}(\mathbf{m}, m_4) \Gamma_{CD} \psi_D^{(f_2),b}(\mathbf{m}, m_4)\, |\Omega\rangle \\
&= \mp \sum_{\mathbf{n},\mathbf{m}} \Gamma_{AB} \Gamma_{CD}\; \langle\Omega|\, \psi_D^{(f_2),b}(\mathbf{m}, m_4) \bar{\psi}_A^{(f_2),a}(\mathbf{n}, n_4)\; \psi_B^{(f_1),a}(\mathbf{n}, n_4) \bar{\psi}_C^{(f_1),b}(\mathbf{m}, m_4)\, |\Omega\rangle\,. \qquad (3.15)
\end{aligned}
$$

Interchanging the Grassmann-valued fermion fields yields an overall minus sign.

The fermionic path integral factorizes into two separate integrations for each flavor $f_i$ that can be performed independently. In principle this step is equivalent to the application of Wick's theorem [1]:

$$\langle \psi_A^a(\mathbf{m}, m_4)\bar{\psi}_B^b(\mathbf{n}, n_4)\rangle_F = \frac{1}{Z_F}\int \mathcal{D}[\psi]\mathcal{D}[\bar{\psi}]\ \psi_A^a(\mathbf{m}, m_4)\bar{\psi}_B^b(\mathbf{n}, n_4)\ e^{-S_F[\psi,\bar{\psi},U]} \tag{3.16}$$

$$= (D^{-1})_{AB}^{ab}(\mathbf{m}, m_4; \mathbf{n}, n_4). \tag{3.17}$$

$S_F$ denotes the fermion action that is of form (2.14), i.e., quadratic in the quark fields. It depends on the gauge field as well. $Z_F$ is the fermionic partition sum and $D^{-1}$ the inverse Dirac or propagator that has components in color and Dirac space. After performing this step only the path integral over the gauge field remains [1]:

$$\left\langle \ ... \ \right\rangle_U \equiv \frac{1}{Z_U}\int \mathcal{D}[U]\ ...\ \det\left(D^{(f_1)}[U]\right)\det\left(D^{(f_2)}[U]\right)e^{-S_U[U]}, \tag{3.18}$$

where $\det\left(D^{(f)}\right)$ denotes the fermion determinant, i.e., the determinant of the Dirac operator depending on the gauge field $U$. The partition function $Z_U$ contains the fermion determinants as well. This yields for the correlator:

$$\begin{aligned} C(n_4 - m_4) &= \mp\sum_{\mathbf{n},\mathbf{m}}\ \Gamma_{AB}\Gamma_{CD}\ \left\langle (D^{-1(f_2)})_{DA}^{ba}(\mathbf{m}, m_4; \mathbf{n}, n_4)(D^{-1(f_1)})_{BC}^{ab}(\mathbf{n}, n_4; \mathbf{m}, m_4)\right\rangle_U \\ &= \mp\sum_{\mathbf{n},\mathbf{m}}\ \left\langle (D^{-1(f_2)})_{DA}^{ba}(\mathbf{m}, m_4; \mathbf{n}, n_4)\Gamma_{AB}\ (D^{-1(f_1)})_{BC}^{ab}(\mathbf{n}, n_4; \mathbf{m}, m_4)\Gamma_{CD}\right\rangle_U \\ &= \mp\sum_{\mathbf{n},\mathbf{m}}\ \left\langle \mathrm{Tr}\left[(D^{-1(f_2)})(\mathbf{m}, m_4; \mathbf{n}, n_4)\Gamma\ (D^{-1(f_1)})(\mathbf{n}, n_4; \mathbf{m}, m_4)\Gamma\right]\right\rangle_U . \end{aligned} \tag{3.19}$$

The big trace $\mathrm{Tr}[\,...\,]$ acts in Dirac and color space.

At this point starts the numerical work. The path integral over the gauge field is on a finite lattice nothing more like a high dimensional integration. Such an integral can be calculated as average over samples of the gauge field, so called configurations. The samples are usually obtained from methods using Markov chain Monte Carlo algorithms [1].

Another difficulty is the numerical handling of the quark propagators. On the lattice the Dirac operator of flavour $f$ is a very large quadratic complex matrix with following number of rows:

$$L_1 \times L_2 \times L_3 \times L_4 \times 3 \times 4\ .$$

Consider a rather small lattice that has spatial dimension $L = 24$ and temporal dimension $T \equiv L_4 = 48$. The Dirac operator $D^{(f)}$ then has $\approx 63 \cdot 10^{12}$ complex entries. To obtain the propagator, $D^{(f)}$ has to be inverted what can not be done for such a large matrix in a reasonable amount of time. Additionally the propagator has to be stored what is inconvenient since it corresponds to 1,014 terabytes of data even for the rather small lattice.

One common method is the computation of so called point-to-all propagators [7]. A point-to-all propagator describes the quark propagation from one fixed lattice site to all other sites. The costs of this simplification appear as large statistical errors of computed quantities.

# 4. Distillation

Distillation is a method of constructing hadron creation operators using eigenvectors of the gauge covariant lattice Laplacian. Distillation is of interest because it enables the computation of all-to-all quark propagators. Furthermore the method is well suited for the observation of ground states of mesonic spectra. Distillation was first proposed in 2009 by Michael Peardon [8].

**Notation:** Variables in square brackets such as $[t]$ are not understood as true variables implying a real functional dependence but more as labels to enumerate expressions.

## 4.1. The lattice Laplacian

The discrete gauge-covariant Laplacian $\triangle$ is a linear, negative-definite and hermitian operator acting on a $M$ dimensional Hilbert space $\mathcal{H} = \mathbb{C}^M$. The Laplacian is defined on a time slice $t$ and the corresponding eigenvalue equation on a particular time slice reads:

$$\triangle\, |v^{(k)}\rangle = \lambda^{(k)}\, |v^{(k)}\rangle\ , \qquad\qquad \lambda^{(k)} \in (-\infty, 0]. \tag{4.1}$$

The label $k$ denotes the number of eigenvalues and eigenvectors. Due to hermiticity and negative semi-definiteness the Laplacian has real and strict negative eigenvalues. The eigenvectors of $\triangle$ are orthogonal and one can find an orthonormal basis of $\mathbb{C}^M$ spanned by the normalised eigenvectors:

$$\sum_{k=1}^{M} |v^{(k)}\rangle\, \langle v^{(k)}| = 1, \qquad\qquad \langle v^{(j)}|v^{(k)}\rangle = \delta_{jk}. \tag{4.2}$$

The eigenequation can be rewritten in position space, i.e., on the lattice as follows:

$$\sum_{\mathbf{n}} \triangle(\mathbf{m};\mathbf{n})[t]\, v^{(k)}(\mathbf{n})[t] = \lambda^{(k)}[t]\, v^{(k)}(\mathbf{m})[t]. \tag{4.3}$$

This equation is solved numerically on every time slice $t$ independently, hence $v^{(k)}(\mathbf{m})[t]$ denotes the $k$-th eigenvector computed on time slice $t$ that corresponds to the eigenvalue $\lambda^{(k)}[t]$ on this particular time slice. The operator can be implemented on the lattice using a symmetric choice for the second derivative:

$$\triangle(\mathbf{m};\mathbf{n})[t] = \sum_{\mu=1}^{3} \Big( U_\mu^\dagger(\mathbf{n}-\hat{\mu}, t)\ \delta_{\mathbf{m},\mathbf{n}-\hat{\mu}} - 2\delta_{\mathbf{m},\mathbf{n}} + U_\mu(\mathbf{n}, t)\ \delta_{\mathbf{m},\mathbf{n}+\hat{\mu}} \Big). \tag{4.4}$$

(4.4) is a $M \times M$ matrix acting on $\mathbb{C}^M$. Here $M$ is defined as $M \equiv L_1 \times L_2 \times L_3 \times N_c$ where $N_c = 3$ denotes the number of colors. In the lattice notation the completeness relation reads as:

$$\sum_{k=1}^{M} v^{(k)}(\mathbf{m})[t] \left(v^{(k)}(\mathbf{n})[t]\right)^\dagger = \delta_{\mathbf{m},\mathbf{n}}. \tag{4.5}$$

Because the gauge covariant Laplacian has color components its eigenvectors have color components as well. Using this fundamental properties of the lattice Laplacian Distillation can be motivated from Gaussian smearing.

## 4.2. The distillation operator

An established smearing technique that is used to increase the contribution of the ground state to the correlator (3.11) is the so called *Gaussian smearing* [8, 9]. Gaussian smearing works by the iterative application of the smearing operator $J_n$ on the quark fields:

$$J_n = \left(1 - \frac{\sigma\triangle}{n}\right)^n, \qquad \sigma \in [0, \infty). \tag{4.6}$$

$n$ denotes the smearing step and $\sigma$ is the smearing parameter. $\triangle$ is the gauge-covariant Laplacian (4.4), hence the smearing preserves gauge symmetry. Since $\triangle$ acts only within time slice $t$, only the spatial part of the quark fields is smeared by applying $J_n$. For a large number of iterations one can rewrite the smearing operator:

$$\begin{aligned} \lim_{n\to\infty} J_n &= e^{\sigma\triangle} \\ &\equiv J. \end{aligned} \tag{4.7}$$

Distillation can be motivated from Gaussian smearing by expanding $J$ in the eigenbase of of the lattice Laplacian using the completeness relation (4.2):

$$\begin{aligned} J &= \sum_{k=1}^{M} |v^{(k)}\rangle \langle v^{(k)}| \, J \\ &= \sum_{k=1}^{M} |v^{(k)}\rangle \langle v^{(k)}| \, e^{\sigma\triangle} \\ &= \sum_{k=1}^{M} |v^{(k)}\rangle \langle v^{(k)}| \, e^{\sigma\lambda^{(k)}}. \end{aligned} \tag{4.8}$$

Since the eigenvalues of $\triangle$ are negative and it is $|\lambda^{(k+1)}| > |\lambda^{(k)}|$ one can see that higher eigenmodes are suppressed exponentially. Hence some number $N \ll M$ can be found such that $\exp(\sigma\lambda^{(N)}) \ll 1$, thus higher eigenmodes can be neglected:

$$J \approx \sum_{k=1}^{N} |v^{(k)}\rangle \langle v^{(k)}| \, e^{\sigma\lambda^{(k)}}. \tag{4.9}$$

This observation is the motivation to *define* [8] the *distillation operator* that inherits a smearing property similar to the Gaussian smearing operator $J$:

$$\begin{aligned} \Box &\equiv \sum_{k=1}^{M} |v^{(k)}\rangle \langle v^{(k)}| \, \theta(|\lambda^{(N)}| - |\lambda^{(k)}|) \\ &= \sum_{k=1}^{N} |v^{(k)}\rangle \langle v^{(k)}| \, . \end{aligned} \tag{4.10}$$

$\theta(x)$ denotes the Heaviside step function. Hence, distillation is also referred to as *LapH smearing* which is an abbreviation for "Laplacian Heaviside".

As well as the Gaussian smearing operator $J$ the distillation operator acts on a time slice $t$. $\Box$ is a projection operator into $\mathbb{C}^N$, i.e., the subspace of $\mathbb{C}^M$ that is spanned by the $N$ lowest eigenvectors. Hence it is $\Box^2 = \Box$. Furthermore (4.10) becomes the completeness relation of the eigenstates for $N = M$, i.e., $\Box = 1$ for $N = M$. The distillation operator can be written as well as a matrix product:

$$\Box[t] = V[t]V^\dagger[t], \tag{4.11}$$

where $V[t]$ is an $M \times N$ matrix whose $k$-th column contains the eigenvector of (4.4) corresponding to the $k$-th lowest eigenvalue on time slice $t$. Writing out the lattice components this expression reads:

$$\Box(\mathbf{m},\mathbf{n})[t] = \sum_{k=1}^{N} v^{(k)}(\mathbf{m})[t] \left(v^{(k)}(\mathbf{n})[t]\right)^\dagger. \tag{4.12}$$

Quark fields that are smeared by applying the distillation operator are also referred to as *distilled fields*:

$$\chi^{(f)}(\mathbf{m},t) \equiv \sum_{\mathbf{n}} \Box(\mathbf{m},\mathbf{n})[t]\psi^{(f)}(\mathbf{n},t). \tag{4.13}$$

The distilled fields $\chi(n)$ inherit all symmetry properties of the unsmeared fields $\psi(n)$ [8], hence the corresponding meson creation operators do so as well.

## 4.3. Meson correlation functions of distilled fields

Meson creation operators like (3.4) can be constructed from distilled quark fields:

$$\begin{aligned}\tilde{O}(t) &= \sum_{\mathbf{m}} \bar{\chi}^{(f_1)}(\mathbf{m},t)\Gamma\chi^{(f_2)}(\mathbf{m},t) \\ &= \sum_{\mathbf{m}}\sum_{\mathbf{n}_1}\sum_{\mathbf{n}_2} \bar{\psi}^{(f_1)}(\mathbf{n}_1,t)\Box(\mathbf{m},\mathbf{n}_1)[t]\ \Gamma\ \Box(\mathbf{m},\mathbf{n}_2)[t]\psi^{(f_2)}(\mathbf{n}_2,t),\end{aligned} \tag{4.14}$$

$$\begin{aligned}\tilde{O}^\dagger(t) &= \pm\sum_{\mathbf{m}} \bar{\chi}^{(f_2)}(\mathbf{m},t)\Gamma\chi^{(f_1)}(\mathbf{m},t) \\ &= \pm\sum_{\mathbf{m}}\sum_{\mathbf{n}_1}\sum_{\mathbf{n}_2} \bar{\psi}^{(f_2)}(\mathbf{n}_1,t)\Box(\mathbf{m},\mathbf{n}_1)[t]\ \Gamma\ \Box(\mathbf{m},\mathbf{n}_2)[t]\psi^{(f_1)}(\mathbf{n}_2,t).\end{aligned} \tag{4.15}$$

The temporal correlation function of these creation operators is:

$$\begin{aligned}C(t'-t) &= \langle\Omega|\,\tilde{O}^\dagger(t')\tilde{O}(t)\,|\Omega\rangle \\ &= \langle\Omega|\,\bar{\psi}^{(f_2)}(\mathbf{n}_1,t')\Box(\mathbf{m}_1,\mathbf{n}_1)[t']\ \Gamma\ \Box(\mathbf{m}_1,\mathbf{n}_2)[t']\psi^{(f_1)}(\mathbf{n}_2,t') \\ &\quad\times\bar{\psi}^{(f_1)}(\mathbf{n}_3,t)\Box(\mathbf{m}_2,\mathbf{n}_3)[t]\ \Gamma\ \Box(\mathbf{m}_2,\mathbf{n}_4)[t]\psi^{(f_2)}(\mathbf{n}_4,t)\,|\Omega\rangle\,,\end{aligned} \tag{4.16}$$

where is an implied summation over all repeated spatial arguments.

In the notation of matrix vector multiplication just writing time indices the correlator can be written as well as:

$$C(t'-t) = \langle\Omega|\, \bar{\psi}^{(f_2)}(t')\Box[t']\,\Gamma\,\Box[t']\psi^{(f_1)}(t') \;\; \bar{\psi}^{(f_1)}(t)\Box[t]\,\Gamma\,\Box[t]\psi^{(f_2)}(t)\,|\Omega\rangle\,. \tag{4.17}$$

Now the same steps as for (3.14) can be performed to rewrite the correlator. Using the expression (4.11) for the distillation operator the correlator reads after performing the fermionic path integral [8]:

$$C(t'-t) = \left\langle \mathrm{Tr}\left[\tau^{(f_2)}[t',t]\tilde{\Gamma}[t]\tau^{(f_1)}[t,t']\tilde{\Gamma}[t']\right]\right\rangle_U, \tag{4.18}$$

where the following definitions have been used:

$$\tilde{\Gamma}_{AB}[t] \equiv V^\dagger[t]\Gamma_{AB}V[t], \tag{4.19}$$

$$\underbrace{\tau^{(f_2)}_{AB}[t',t]}_{N\times N} \equiv \underbrace{V^\dagger[t']}_{N\times M}\underbrace{(D^{-1(f_2)})_{AB}(t';t)}_{M\times M}\underbrace{V[t]}_{M\times N}, \qquad \tau^{(f_1)}_{AB}[t,t'] \equiv V^\dagger[t](D^{-1(f_1)})_{AB}(t;t')V[t']. \tag{4.20}$$

$A$ and $B$ denote spin indices. $\tau[t',t]$ is the reduced propagator or *perambulator*; it contains the complete information of the corresponding quark's propagation from every spatial point on time slice $t$ to any spatial point on time slice $t'$. $\tau_{AB}[t',t]$ is a complex $N\times N$ matrix, where $N$ is the number of eigenvectors used to construct the distillation operator. Since it is $N \ll M$ the perambulator can be computed in a reasonable amount of time.

(4.18) reveals a further useful property [8] of the distillation method: The perambulators $\tau^{(f)}[t',t]$ that contain the information about the quark propagation and $\tilde{\Gamma}[t]$ that contains the quantum numbers of the meson under investigation can be computed independently. This means that perambulators once computed and stored can be reused to observe different mesons simply by combining the existing $\tau^{(f)}[t',t]$'s with different $\tilde{\Gamma}[t]$'s carrying the quantum numbers of interest.

## 4.4. Computation of the propagators

In order to obtain the propagator the Dirac operator, that is a large matrix on the lattice, has to be inverted. The propagator is defined by the equation:

$$\sum_{\mathbf{u},u_0}(D^{(f)})^{ab}_{AB}(\mathbf{m},m_0;\mathbf{u},u_0)\;(D^{-1(f)})^{bc}_{BC}(\mathbf{u},u_0;\mathbf{n},n_0) = \delta_{a,c}\delta_{A,C}\delta_{m_0,n_0}\delta_{\mathbf{m},\mathbf{n}}. \tag{4.21}$$

Numerically one does not calculate the entire propagator at once but so called *inversions* $\Phi(m)$ that correspond to single columns of the propagator in the case of point-to-all propagators [7]. Thus, the inversion $\Phi(m)$ is *defined* to be the solution of the following linear equation system:

$$\sum_{\mathbf{m},m_0}(D^{(f)})^{ab}_{AB}(\mathbf{n},n_0;\mathbf{m},m_0)\;\Phi^{(f),b}_B(\mathbf{m},m_0) = \xi^a_A(\mathbf{n},n_0) \tag{4.22}$$

$$\Leftrightarrow \Phi^{(f),a}_A(\mathbf{m},m_0) = \sum_{\mathbf{n},n_0}(D^{-1(f)})^{ab}_{AB}(\mathbf{m},m_0;\mathbf{n},n_0)\;\xi^b_B(\mathbf{n},n_0). \tag{4.23}$$

$\xi(n)$ is the so called *source* that is, as well as $\Phi(m)$, a fermionic field with color components.

The inversions $\Phi(m)$ of the Dirac operator are calculated under the specification of a special type of sources $\xi(n)$ [7]. This approach can as well be used to compute the perambulators (4.20).

The goal is to obtain the sources $\xi(n)$ that have to be specified to calculate inversions corresponding to single columns of the perambulator $\tau^{(f)}_{AB}[t,t']$. In order to do so the perambulator can be rewritten:

$$\begin{aligned}
&\tau^{(f)}_{A'B'}[t,t'] = V^\dagger[t]\ (D^{-1(f)})_{A'B'}(t,t')V[t'] \\
&= \sum_{k=1}^{N}\sum_{\mathbf{m},\mathbf{n}} (v^\dagger)^{(k),a}(\mathbf{m})[t]\ (D^{-1(f)})^{ab}_{A'B'}(\mathbf{m},t;\mathbf{n},t')\ v^{(k),b}(\mathbf{n})[t'] \\
&= \sum_{k=1}^{N}\sum_{\mathbf{m},\mathbf{n}} (v^\dagger)^{(k),a}(\mathbf{m})[t]\ \delta_{A,'A}\ (D^{-1(f)})^{ab}_{AB}(\mathbf{m},t;\mathbf{n},t')\ v^{(k),b}(\mathbf{n})[t']\ \delta_{B,B'} \\
&= \sum_{k=1}^{N}\sum_{\mathbf{m}}\sum_{\mathbf{n},n_0} (v^\dagger)^{(k),a}(\mathbf{m})[t]\ \delta_{t,m_0}\delta_{A,'A}\ (D^{-1(f)})^{ab}_{AB}(\mathbf{m},m_0;\mathbf{n},n_0)\ v^{(k),b}(\mathbf{n})[t']\ \delta_{t',n_0}\delta_{B,B'}. \qquad (4.24)
\end{aligned}$$

Now, the expression for the inversion can be identified from (4.24):

$$\Phi^{(f),a}_{A}(\mathbf{m},m_0)[t',B',k] \equiv \sum_{\mathbf{n},n_0} (D^{-1(f)})^{ab}_{AB}(\mathbf{m},m_0;\mathbf{n},n_0)\ v^{(k),b}(\mathbf{n})[t']\ \delta_{t',n_0}\delta_{B,B'}. \qquad (4.25)$$

$\Phi(m)[t',B',k]$ is the an object with color and spin components on every lattice point. The label $[t',B',k]$ means that $\Phi(m)[t',B',k]$ is defined on time slice $t'$, spin index $B'$ for the $k$-th eigenvector. Now the source term that has to be specified to obtain $\Phi(m)[t',B',k]$ can be read off comparing (4.25) and (4.23):

$$\xi^b_B(\mathbf{n},n_0)[t',B',k] = v^{(k),b}(\mathbf{n})[t']\ \delta_{t',n_0}\delta_{B,B'}. \qquad (4.26)$$

In order to obtain all inversions to build the entire matrix $\tau[t',t]$ one has to compute $L_4 \times 4 \times N$ inversions $\Phi(m)[t',B',k]$ for all values of $[t',B',k]$. Thus, the same number of sources of type (4.26) has to be generated.

For this work sources of type (4.26) have been generated and stored. The files containing the data of a single source have been submitted to the program `tmLQCD` [10] that executes the computation of the corresponding inversions. Details of the implementation are described in section 5.

## 4.5. Problems of distillation

In order to create a picture close to physical reality it is necessary to implement mesons on the lattice with some finite spatial extension corresponding to the physical size of a meson that is 1fm in diameter. Local meson creation operators like (3.1) are not adequate since they create a meson on one particular lattice point, i.e., without any spatial extension. Meson operators creating spatially extended mesons are obtained from the use of quark fields spatially smeared by the action of the Gaussian smearing operator (4.7). It is called "Gaussian" smearing because the smeared quark wave function is of Gaussian shape. Distillation provides a spatial smearing of quark wave functions with Gaussian shape as well. By removing eigenmodes from (4.10), the spatial extension of the smeared field is increased.

An unsmeared quark state $|\psi\rangle$ is localised at one lattice point, i.e., the spatial wave function $\psi(\mathbf{n}) = \langle \mathbf{n}|\psi\rangle$ is very narrow in its spatial extension. $|\psi\rangle$ can be expanded in the basis spanned by the eigenmodes of the lattice Laplacian:

$$\begin{aligned} |\psi\rangle &= \sum_{k=1}^{M} |v^{(k)}\rangle \langle v^{(k)}|\psi\rangle \\ \Leftrightarrow \psi(\mathbf{n}) &= \sum_{k=1}^{M} \langle \mathbf{n}|v^{(k)}\rangle \langle v^{(k)}|\psi\rangle \,. \end{aligned} \tag{4.27}$$

By removing higher eigenmodes of the lattice Laplacian the completeness relation becomes the distillation operator (4.10). The more eigenmodes are removed the lager becomes the width of the wave function $\psi(\mathbf{n})$.

A helpful analogy is to think of distillation as a kind of Fourier decomposition where some state $|f\rangle$ is expanded in the eigenmodes of some differential operator $D\,|k\rangle = ik\,|k\rangle$:

$$\begin{aligned} |f\rangle &= \sum_{k} |k\rangle \langle k|f\rangle \\ \Leftrightarrow f(x) &= \sum_{k} \langle x|k\rangle \langle k|f\rangle \\ &\sim \sum_{k} \tilde{f}_k \cdot e^{ikx}. \end{aligned} \tag{4.28}$$

Thinking of $f(x)$ as a Gaussian wave packet, a large number of $k$-modes has to be added up in order to obtain a well localized wave packet.

The same is true for distillation: In order to obtain a Gaussian shaped quark wave function $\psi(\mathbf{n})$ whose spatial extension resembles the size of a meson (1fm) a large number of eigenmodes has to be added to the distillation operator (4.10). If the number of included eigenmodes is to low, the corresponding quark wave function is extended over the entire spatial lattice (2-4fm). The overlap of this state and the actual ground state would be small.

The computation of a sufficient number of eigenvectors in order to obtain a suitable quark wave function is related to major computational efforts. But on the other hand, the possibility of computing to all-to-all quark propagators is a profit since physical information is preserved and noise of the correlation signal can be reduced [11].

# 5. Implementation and documentation

In this section some details of the implementation of the generation of the inversions (4.24) are provided. The process of computing the inversions can be split in three sequential steps that are:

- the computation of the desired number $N$ of eigenvectors
- the generation of $L_4 \times 4 \times N$ sources (4.26) using the computed eigenvectors
- the computation of the inversions (4.25)

For the implementation modules of the contraction code package written by the ETM Collaboration are used as well as the `tmLQCD` package [10].

## 5.1. Lattice setup

The gauge field configurations used for the calculations as part of this thesis are obtained from the ensemble A40.24 [12]. The ensemble has been generated using $N_f = 2 + 1 + 1$ quark flavours: mass-degenerate up and down and mass-split strange and charm quarks. Details of the used fermion and gauge actions can be looked up in [12]. The gauge configurations are characterized by the following set of parameters:

| # of used configurations | $\beta$ | $\kappa$ | $a\mu_l$ | $a\mu_\sigma$ | $a\mu_\delta$ | $(L/a)^3 \times T/a$ |
|---|---|---|---|---|---|---|
| 11 | 1.9 | 0.1632700 | 0.0040 | 0.150 | 0.190 | $24^3 \times 48$ |

Table 4: Parameters of used gauge configurations

$a$ denotes the lattice spacing, $\beta$ the gauge coupling (2.12), $\kappa$ is the hopping parameter (2.16), $\mu_l$ is the twisted mass of the light doublet $\chi_l = (\chi^{(u)}, \chi^{(d)})$. $\mu_\sigma$ and $\mu_\delta$ are twisted mass parameters as well that arise from the fermion action that was used for the heavy doublet $\chi_h = (\chi^{(s)}, \chi^{(c)})$.

In this simulation sea quarks have flavours up, down, strange and charm while valence quarks are just of the flavours up and down.

## 5.2. Performed computations

The computations that are performed for this thesis are:

- computation of $N = 5$ eigenvectors of the lattice Laplacian on every lattice time slice for all 11 gauge configurations
- computation of $48 \times 4 \times 5$ distillation sources on each of the 11 configurations
- computation of the $48 \times 4 \times 5$ inversions on each of the 11 configurations

The steps consuming the most computation time are the computation of the eigenvectors and the computation of the inversions. Whereas the generation of the distillation sources can be done quite fast. Details of the implementations of each step are provided in the next subsections.

## 5.3. Added modules

Modules written for this work are added to the contraction code in the directory `/.../Distillation/`. The new modules are:

- `/Distillation/generate_distillation_source/`: contains the function that generates one distillation source (4.26) for given values $[t', B', k]$
- `/Distillation/eigenvector_utils/check_eigenvector/`: contains a function that checks if a passed eigenvector fulfills the eigenequation of the Laplacian (4.4)

- `/Distillation/eigenvector_utils/sort_eigenvectors/`: contains a function that sorts the eigenvalues of a submitted eigenvector by increasing magnitude and arranges the corresponding eigenvectors in the storage according to this order
- `/Distillation/eigenvector_utils/linear_algebra_operations/`: contains a set of auxiliary functions that perform linear algebra operations used to work with the eigenvectors

The modules listed above are written in the programming language C. Functions that may be reused by others can be accessed by including the following header files:

- `/Distillation/generate_distillation_source/generate_distillation_source.h`
- `/Distillation/eigenvector_utils/check_eigenvector/check_eigenvector.h`
- `/Distillation/eigenvector_utils/sort_eigenvectors/sort_eigenvectors.h`
- `/Distillation/eigenvector_utils/linear_algebra_operations/linear_algebra_operations.h`

The parameters of each function declared in one of this `.h`-files are explained via a comment within the respective `.h`-file.

## 5.4. Computation of eigenvectors

For the computation of eigenvectors code written for older projects [13, 14] is reused. Using this code a main source file for the eigenvector computation has been written:

- `/Distillation/calc_eigenvectors.c`

The corresponding executable can be run in the command line via:

```
./calc_eigenvectors </path/to/config> </path/to/vector/> <T> <L> <gauge_field_id>
    <total_number_eigenvectors>
```

where the following input parameters have to be specified:

- `</path/to/config>`: total path of config. file on that eigenvectors are shall be computed
- `</path/to/vector/>`: total path to the directory where one wants to store the vector
- `<T>`: temporal extension of the lattice
- `<L>`: spatial extension of the lattice
- `<gauge_field_id>`: ID of gauge configuration, i.e., the file extension of the config. file
- `<total_number_eigenvectors>`: the total number of eigenvectors one wants to compute, i.e., $N$

The program solves the eigenvalue equation of the Laplacian on every time slice of the lattice and stores the eigenvectors of all timeslices together with the corresponding eigenvalues in a single block of data. This data block is written into an output file whose file extension is the ID of the gauge configuration on that the eigenvectors are calculated [14].

## 5.5. Generation of sources

The source code that contains the main function that executes the calculation of the distillation sources (4.26) is:

- `/Distillation/generate_distillation_sources.c`

The corresponding executable can be run in the command line via:

```
./generate_distillation_sources </path/to/vector> <gauge_field_id> </path/to/source/> <T>
    <L> <total_number_eigenvectors>
```

The parameters not explained explicitly are the same as for the eigenvector program:

- `</path/to/vector>`: total path of file that contains eigenvector used to generate the sources
- `<gauge_field_id>`: ID of gauge field the eigenvector was computed on
- `</path/to/source/>`: total path to the directory where one wants to store the sources

This program generates $T \times 4 \times N$ sources from all $T \times N$ eigenvectors that have been computed on one particular gauge configuration.

## 5.6. Computation of inversions

In order to compute the inversions (4.25) the `tmLQCD` package [10] ("twisted mass Lattice QCD") has been used. The package is available on GitHub[1]. It provides the so called inverter, a program that computes inversions (4.23) for submitted sources $\xi(n)$ on a given gauge configuration.

During the build process of the `tmLQCD` package there is created a directory called `.../bin/` inside the installation directory. `.../bin/` contains the executable of the inverter `.../bin/invert`. The inverter can be run in the command line by submitting an inverter job script:

```
./invert -f inverter_script.input
```

An example of an invert job script is provided in Fig.4. The physical parameters that have to be specified in `inverter_script.input` arise from the Dirac operator that shall be inverted. The parameters for computation are listed in Tab. 4:

- `2KappaMu = 0.00130616` $= 2 \cdot \kappa \cdot \mu_l$
- `kappa = 0.1632700`

The calculated inversions correspond to the Dirac operator that arises from the Wilson twisted mass action (2.16) for the light quark flavours $u$ and $d$. Since the twisted mass quarks are mass degenerate inversions of flavour $u$ and $d$ are the same.

For every gauge configuration of the given ensemble $T \times 4 \times N$ distillation sources have to be submitted to the inverter in order to obtain the same number of inversions.

[1] `https://github.com/etmc/tmLQCD`

```
L=24
T=48

2KappaMu = 0.00130616
CSW = 1.0
kappa = 0.1632700
DebugLevel = 3
InitialStoreCounter = 249
seed = 6098312
Measurements = 1
ThetaT = 1.0
GaugeConfigInputFile = /path/to/configs/conf
UseEvenOdd = yes
UseRelativePrecision = yes
ReproduceRandomNumbers = yes
RanluxdLevel = 2
SourceFilename = /path/to/source/source.0750
ReadSource = yes
SplittedPropagator = no
Measurements = 1
Indices = 0
DisableIOChecks = yes
DisableSourceIOChecks = yes

BeginOperator TMWILSON
2kappaMu = 0.00130616
kappa = 0.1632700
SolverPrecision = 1e-24
MaxSolverIterations = 20000
AddDownPropagator = no
EndOperator
```

Figure 4: Inverter script `inverter_script.input`

# 6. Conclusions and outlook

The computations of the inversions are the first step in order to compute a meson mass. The next step towards the meson mass is the computation of the correlator (4.18) using the generated inversions. The correlator of any meson consisting of up and down valence quarks can be computed by combining the inversions with a $\tilde{\Gamma}$ (4.19) carrying the quantum numbers of the meson one likes to observe.

This work constitutes a first step of a test of distillation by our work group with the aim to collect first experience in working with this method. Hence the setup is kept simple by using a small set of configurations and a small number of eigenvectors of the Laplace operator. Further, the eigenvectors are computed for the sake of simplicity on unsmeared gauge configurations. The implementation of a gauge field smearing is a further step for future projects in order to obtain better correlation signals. The low number of used eigenvectors results in widely smeared meson states. Hence a larger number $\mathcal{O}(100)$ of eigenvectors should be used to improve the computations's quality.

# Bibliography


[1] Christof Gattringer and Christian B. Lang. Quantum chromodynamics on the lattice. *Lect. Notes Phys.*, 788:1–343, 2010.

[2] Joshua Ellis. TikZ-Feynman: Feynman diagrams with TikZ. 2016.

[3] Y. Iwasaki, K. Kanaya, T. Kaneko, and T. Yoshie. Scaling in SU(3) pure gauge theory with a renormalization group improved action. *Phys. Rev.*, D56:151–160, 1997.

[4] Andrea Shindler. Twisted mass lattice QCD. *Phys. Rept.*, 461:37–110, 2008.

[5] Marc Wagner, Stefan Diehl, Till Kuske, and Johannes Weber. An introduction to lattice hadron spectroscopy for students without quantum field theoretical background. 2013.

[6] Stephan Güsken. A study of smearing techniques for hadron correlation functions. *Nuclear Physics B - Proceedings Supplements*, 17:361 – 364, 1990.

[7] Abdou Abdel-Rehim, Constantia Alexandrou, Joshua Berlin, Mattia Dalla Brida, Jacob Finkenrath, and Marc Wagner. Investigating efficient methods for computing four-quark correlation functions. 2017.

[8] Michael Peardon, John Bulava, Justin Foley, Colin Morningstar, Jozef Dudek, Robert G. Edwards, Balint Joo, Huey-Wen Lin, David G. Richards, and Keisuke Jimmy Juge. A Novel quark-field creation operator construction for hadronic physics in lattice QCD. *Phys. Rev.*, D80:054506, 2009.

[9] Karl Jansen, Chris Michael, Andrea Shindler, and Marc Wagner. The Static-light meson spectrum from twisted mass lattice QCD. *JHEP*, 12:058, 2008.

[10] K. Jansen and C. Urbach. tmLQCD: A Program suite to simulate Wilson Twisted mass Lattice QCD. *Comput. Phys. Commun.*, 180:2717–2738, 2009.

[11] Justin Foley, K. Jimmy Juge, Alan O'Cais, Mike Peardon, Sinead M. Ryan, and Jon-Ivar Skullerud. Practical all-to-all propagators for lattice QCD. *Comput. Phys. Commun.*, 172:145–162, 2005.

[12] R. Baron et al. Light hadrons from lattice QCD with light (u,d), strange and charm dynamical quarks. *JHEP*, 06:111, 2010.

[13] Janik Kämper. Non-string-like trial states for static potential computations. 2014.

[14] Tobias Neitzel. Computation of the static quark-antiquark potential using non-string-like trial states. 2015.

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## Selbstständigkeitserklärung

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

Hiermit erkläre ich, dass ich die Arbeit selbststädig 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 kentlich gemacht worden. Ferner erkläre ich, dass die Arbeit nicht - auch nicht auszugsweise - für eine andere Prüfung verwendet wurde.

Ort, Datum

Jan Kruse