The pion Form Factor from Lattice QCD
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Chapter 5.

Analysis of the three-point function: extraction of the form factor at $T = 0$

In Chapter 4 we have studied properties of the pion extracted from the two-point function. This correlation function is especially suited for the determination of masses, energies and properties related to them, but less for the investigation of the electromagnetic structure; the charge radius we extracted there was at best a qualitative estimate. In this Chapter we will present results based on the three-point function, i.e. the $\gamma\pi\pi$ vertex. We will extract the pion charge form factor, a central result of this work. From this form factor, we can compute the mean square radius in an entirely different, and more meaningful fashion. We start this chapter with the parametrisation of the form factor and the three-point correlator. The extraction techniques are discussed, followed by the results for the various observables. Special attention is given to the charge radius, since it is an observable for which one has some guidance for the extrapolation to the physical limit and it is therefore suitable for comparison with experimental data.

5.1. Form factor of the free pion

As already mentioned in the Introduction, the form factor can be extracted from the matrix element for the pion-photon interaction. In the continuum it is given by

$$\Gamma_\mu = \langle \pi(p_f)|j_\mu(0)|\pi(p_i)\rangle_{\text{cont}} \quad (5.1)$$

For the free pion (i.e. at zero temperature), the Lorentz decomposition is simple since there are only two independent four-vectors and one scalar variable. The structure thus reads

$$\Gamma_\mu = q_\pi (p_f + p_i)_\mu F(Q^2) + q_\pi q_\mu G(Q^2), \quad (5.2)$$

where we have used $q_\mu = (p_f - p_i)_\mu$ as the photon momentum, and $Q^2 = -q^2$. Current conservation then yields the condition

$$q^\mu \Gamma_\mu = q_\pi q^2 G(Q^2) = 0. \quad (5.3)$$

Since this must hold for all $q^2$, $G(Q^2)$ must vanish and the matrix element can be parametrised with only one form factor

$$\Gamma_\mu = q_\pi (p_f + p_i)_\mu F(Q^2). \quad (5.4)$$
Chapter 5. Analysis of the three-point function: extraction of the form factor at \( T = 0 \)

Taking into account the different normalisations in the continuum and on the lattice

\[
\langle \pi(p_f)|j_\mu(0)|\pi(p_i)\rangle_{\text{Latt.}} = \frac{\langle \pi(p_f)|j_\mu(0)|\pi(p_i)\rangle_{\text{cont}}}{2\sqrt{E_{p_f}^0 E_{p_i}^0}}, \tag{5.5}
\]

we can write for the lattice version of the pion-photon matrix element

\[
\langle \pi(p_f)|j_\mu(0)|\pi(p_i)\rangle_{\text{Latt.}} = q_\pi F(Q^2) \frac{(p_f + p_i)_\mu}{2\sqrt{E_{p_f}^0 E_{p_i}^0}}. \tag{5.6}
\]

### 5.2. Parametrisation

The form factor is non-trivially embedded in the data for the three-point function. We therefore need an appropriate parametrisation to describe its behaviour and extract the desired quantities. The starting point is the momentum-space correlation function, Eq. 3.46, with the integrand

\[
G(x_\tau, x, x_\tau) = \langle \Omega|T(\phi_\pi(x_\tau)j_\mu(x)\phi_\pi^+(x_\tau))|\Omega\rangle. \tag{5.7}
\]

Writing out the time-ordered product, taking into account the boundary conditions of our lattice and choosing \( t_i < t < t_f \), the contributions to this function can be divided in three classes of diagrams: diagrams with only a pion contributing (Fig. 5.1(a)), diagrams also involving a vector-like particle state (Fig. 5.1(b)) and diagrams in which the vacuum is not 'empty' (Fig. 5.1(c)).

Because of translational invariance, the three-point function only depends on two coordinates; the distances \( x_{\tau} - x \) and \( x - x_{\tau} \). Without loss of generality, we therefore choose for simplicity \( x_\tau = (0, 0) \). Although \( p_f, p_i \) and \( q \) are not independent, we will use all three of them for notational convenience.

The diagrams of the first class constitute the main contribution, which in momentum space is given by

\[
\tilde{G}_{\mu,R}(t_f, t; p_f, q) = \int dx_\tau \int dx e^{-ip_\tau \cdot (x_\tau - x) + iq \cdot x} G_\mu(x_\tau, x)
\]

\[
= \sum_{m,n} \langle \Omega|\phi_R|m, p_f\rangle\langle m, p_f|j_\mu(0)|n, p_i\rangle\langle n, p_i|\phi_R^+(0)|\Omega\rangle
\]

\[
\times e^{-E_{p_f}^m (t_f - t)} e^{-E_{p_i}^n t}, \tag{5.8}
\]

where we have again added the subscript \( R \) to denote the smearing level.

Diagrams belonging to the second class arise when the photon acts as a creation operator for vector states; e.g. a rho meson or a state of two pions with the correct angular momentum. For a \( \rho \)-meson, the contribution has the following structure in
5.2. Parametrisation

(a) One of two diagrams belonging to class I.

(b) A typical Diagram belonging to class II.

(c) A diagram belonging to class III. The vacuum is replaced with particle $P$.

Figure 5.1: Different contributions to the three-point function

In addition to the extra vector particle propagator, they thus involve a longer propagation of the pion, which makes them exponentially suppressed with respect to the pure pion diagrams in class I, when $t_f$ is chosen small enough. These are the 'more severe' wrapping around effects mentioned in Sec. 3.3.1, which become important when the condition $t_f \ll N_\tau - t_f$ is not fulfilled. For a simple estimate of this contribution, we assume that its matrix elements are of the same size as the ones appearing in the diagrams of class I. The diagrams of the second class are then exponentially suppressed.
and they are left out of our parametrisation.

The diagrams of the third class are even more exponentially suppressed because of particle $P$ which traverses the complete lattice in the temporal direction. These diagrams will also be neglected in our parametrisation.

Summarising the above considerations, we find that we only need to consider diagrams of class I, Eq. 5.8, since they constitute the dominant contribution to Eq. 3.46.

The pion operators of Eq. 3.20 actually create/annihilate a general pseudo-scalar state. We have used smearing techniques (See Sec. 3.3.1) to enhance the fraction of pions at the sink. Allowing the state to propagate in time further reduces the amount of possible states enormously since most of them are very heavy. The pion is the lightest pseudo scalar, therefore it is safe to assume that only the pion and possible its first excited states contribute to the pion three-point function. Applying this to our parametrisation and using Eq. 5.6 then leads to the following expression

$$
\widetilde{G}_{\mu,R}(t_f, t; p_f, q) = q_\pi F(Q^2) \frac{(p_f + p_i)_\mu}{2} \sqrt{Z_R^0(p_f) Z_R^0(p_i)} e^{-E_{p_f}^0 (t_f - t)} e^{-E_{p_i}^0 t} + \sum_{m,n \neq (0,0)} \sqrt{Z_R^m(p_f) Z_R^m(p_i)} \langle m, p_f | j_\mu(0) | n, p_i \rangle e^{-E_{p_f}^m (t_f - t)} e^{-E_{p_i}^m t}. \quad (5.10)
$$

The $Z$-factors are defined in Eq. 4.5 and $q_\pi$ denotes the pion charge. This parametrisation can be further simplified as will be discussed in Sec. 5.3.

### 5.2.1. Current conservation and the second insertion

The special case of $Q^2 = 0$ needs a discussion on its own, since in this case we can exploit current conservation on the operator level which connects the two- and three-point functions [4,49].

The general time-ordered two-point function for the pion can be written as

$$
G_R^{(2)}(x, y) = \langle \Omega | T(\phi_R(x_f) \phi^{-\dagger}(x_i)) | \Omega \rangle, \quad (5.11)
$$

where we have added here the superscript $2$ to avoid confusion with the three-point function. We choose $t_f > t_i$. Taking into account our periodic boundary conditions, we see that two terms contribute

$$
G_R^{(2)}(x_f) = \langle \Omega | \phi_R(t_f, x_f) \phi^{-\dagger}(t_i, x_i) + \phi^{-\dagger}(N_f + t_i, x_i) \phi_R(t_f, x_f) | \Omega \rangle \quad (5.12)
$$

For the three point function the time-ordered product, without fixing the time com-
ponents of the operator, we have in general
\begin{equation}
G_{\mu, R}(x_f, x, x_i) = \langle \Omega | T(\phi(x_f) j_{\mu}(x) \phi^\dagger(x_i)) | \Omega \rangle = \langle \Omega | \theta(t_f - t) \theta(t - t_i) \phi(x_f) j_{\mu}(x) \phi^\dagger(x_i) + \theta(t_f - t_i) \theta(t_i - t) \phi(x_f) j_{\mu}(x) \phi^\dagger(x_i) + \theta(t - t_f) \theta(t_i - t) \phi(x_f) j_{\mu}(x) \phi^\dagger(x_i) + \theta(t_i - t_f) \theta(t_i - t) \phi(x_f) j_{\mu}(x) \phi^\dagger(x_i) \rangle. \quad (5.13)
\end{equation}

On the operator level the vector current is conserved because of the gauge symmetry. It is given by
\begin{equation}
\partial^\mu j_{\mu} = 0. \quad (5.14)
\end{equation}

From the Noether theorem, we find for the corresponding conserved charge
\begin{equation}
Q = \int d^3x \, j_4(t, x). \quad (5.15)
\end{equation}

This operator has the following properties
\begin{align}
Q \phi^\dagger(x_i) | \Omega \rangle &= q_\pi \phi^\dagger(x_i) | \Omega \rangle, \\
Q \phi(x_f) | \Omega \rangle &= -q_\pi \phi(x_f) | \Omega \rangle, \\
Q | \Omega \rangle &= 0, \\
\langle \Omega | Q &= 0. \quad (5.16)\end{align}

Using these equalities, we are left with only two contributions contributing to the integrated three-point function \((\mu = 4)\)
\begin{equation}
\int d^3x \, G_{4, R}(x_f, x, x_i) = q_\pi \{ \langle \Omega | \theta(t_f - t) \theta(t - t_i) \phi(x_f) \phi^\dagger(x_i) | \Omega \rangle \\
- \langle \Omega | \theta(t_i - t_f) \theta(t - t_f) \phi^\dagger(x_i) \phi(x_f) | \Omega \rangle \}. \quad (5.18)
\end{equation}

The second term on the r.h.s., the so-called second insertion, is a contribution for \(t > t_f\) and arises because of our periodic boundary conditions. It effectively 'measures' the charge of the pion flowing in the negative time direction. This contribution is also exponentially suppressed \((\approx e^{-E(N_r - t_f)} / e^{-Et_f})\), and was not discussed in the previous section, since it is not necessary for the extraction of the form factor away from the photon point due to our particular analysis methods, see Sec. 5.4. In deriving a relation between the two- and three-point function, we however need its contribution.

Since we can calculate the two contributions separately by changing the time coordinate of the current operator in the simulation, we can choose to subtract the second insertion from the first \((t_i < t < t_f)\), thereby obtaining the useful identity
\begin{equation}
\int d^3x \, G_{4, R}(x_f, x, x_i) = q_\pi \langle \Omega | \phi(x_f, x_i) \phi^\dagger(t_i, x_i) + \phi^\dagger(t_i + N_r, x_i) \phi(t_f, x_f) | \Omega \rangle = q_\pi G_R^{(2)}(x_f, x_i) \quad (5.19)\end{equation}
We have used $t_i + N_\tau > t_f > t_i$, the periodic boundary conditions and, in the second term on the r.h.s. of Eq. 5.18, $t_f < t < t_i + N_\tau$ to evaluate the step functions. As in the previous section we choose $t_i = 0$, and observe that the integral over $x$ in Eq. 5.19 is the Fourier transform of variable $x$ for $q = 0$ in Eq. 5.8. Performing the Fourier transform on the other coordinate ($x_f$), we obtain the momentum space relation

$$
\tilde{G}_{4,R}(t_f, t; \mathbf{p}, 0) - \tilde{G}_{4,R}(t_f, t'; \mathbf{p}, 0) = q^f \tilde{G}^{(2)}_R(t_f, \mathbf{p}),
$$

with $t_i < t' < N_\tau$ and $\mathbf{p} = \mathbf{p}_f = \mathbf{p}_i$. This relation between the two- and three-point function ensures that $F(0) = q = 1$. Since current conservation is obeyed on the (fermion) operator level, the identity must hold on a single configuration. By comparing the independently determined r.h.s. and l.h.s., we can test if $F(0) = 1$ and thus assess our numerical accuracy.

5.3. Simulation

As already hinted at in Sec. 5.2, we can simplify the extraction of the form factor considerably by appropriate choices for the kinematics. By inspection of Eq. 5.6, we see that making the choices $|\mathbf{p}_f| = |\mathbf{p}_i|$ and $\mu = 4$, the energy pre-factor reduces to one. Because of the first choice, we have that $E_{p_f}^0 = E_{p_i}^0$ leading to $q_0 = -Q_0 = 0$ and $Q^2 = q^2$. A further consequence of this choice is that the ground-to-ground state contribution, i.e. the first term in Eq. 5.10, doesn’t exhibit a dependence on the insertion time $t$. Observing a time dependence in our data automatically leads us to conclude that excited state contributions are present and thus the second term in Eq. 5.10 must be included in our parametrisation.

The momentum transfer is controlled by varying the angle between the two momenta. We choose $|\mathbf{p}_f| = |\mathbf{p}_i| = p = \sqrt{2}|p_{\text{min}}|$ ($\approx 0.37$), where

$$
|p_{\text{min}}| = \frac{2\pi}{N_\sigma}
$$

is the minimal momentum for a lattice with extent $N_\sigma$ in the spatial direction. This choice enables us to consider five different momentum transfers with only one final state momentum. At the same time the momentum is low enough to ensure continuum kinematics (see Sec. 4.4.5).

Since we want to suppress the diagrams of the second class, i.e., the wrapping around effects, as much as possible, we have to keep the distance between the source and sink small compared to the total extent of the lattice. We choose $t_i = 0$ and $t_f = 11$, leaving $t$ as the only time dependence. The insertion time $t$ will be varied within the domain $[0, t_f]$, but in order to evaluate the second inversion and Eq. 5.20, we also choose some values $t > t_f$.

A last thing to note from the parametrisation in Eq. 5.10 is that the elastic contribution from the excited state ($n = m = 1$) has the same functional dependence as the
5.4. Analysis methods

It is therefore impossible to disentangle the two. We can however estimate the \( n = m = 1 \) term using the excited state energy and amplitude obtained in the previous Chapter. Assuming the two form factors are of the same order of magnitude, the relative contribution is governed by the difference \( E^1 - E^0 (\approx 0.5) \) in the exponent and the ratio of the Z-factors. The relative importance of the elastic excited state is then estimated to be of the order of 1% or less. We therefore neglect this contribution.

The above considerations lead to the following simplified parametrisation of the three-point function

\[
\tilde{G}_{4,R}(t_f, t; p_f, q) = q_{\pi} F(Q^2) \sqrt{Z_R^0(p) Z_0^0(p)} e^{-E^0_{p,t_f}}
\]

\[
+ \left\{ \sqrt{Z_R^0(p) Z_0^1(p)} (0, p_f | j_{\mu}(0) | 1, p_f) e^{-E^0_{p,t_f-t}} e^{-E^1_{p,t_f}} + (1 \rightarrow 0) \right\},
\]

with \( p = |p_f| = |p_i| \). The subscript on the momentum referring to the initial or final state has been dropped when possible.

5.4. Analysis methods

In the previous sections, we discussed the parametrisation of the three-point function for the analysis of the raw data. In this section we focus on the methods for extracting the form factor.

In the earlier work on the pion form factor [5,10], the authors chose to use ratios of three- and two-point functions to extract it. In order to use this method one assumes no contributions of excited states for at least a small region of time, i.e. the onset of a plateau in the three-point function as a function of the insertion time \( t \) (cf. Eq. 5.22) must be visible. In Fig. 5.2 we show typical examples of jackknife datasets for various \( Q^2 \) and masses, based on the improved, Eq. 3.36, and conserved, Eq. 3.33, currents. From these figures, we see that the data clearly indicate the admixture of excited states. Their relative contribution increases for increasing \( Q^2 \) and decreasing mass. For most three-point functions shown in the figure there is no indication of (the onset of) a plateau and thus it is not safe to assume that only the ground state contributes.

Another possibility to extract the form factor is to fit the data using the parametrisation derived in the previous section. There is however no \( t \)-dependence in the term containing the form factor. While we can extract this \( t \)-independent elastic contribution of the ground state, we cannot extract the form factor from the three-point function without prior knowledge of the energy and amplitude of the ground state. One strategy is to first determine these observables from a fit to the two-point function. These can then serve as fixed input parameters in the fit to the three-point function, thus enabling us to obtain the form factor.

The jackknife sets are averages over a large part of the data sample and thus the correlations are to a large extent averaged out. However, fluctuations between the sets
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and correlations between the two Green's functions are still present. These fluctuations increase with e.g. decreasing mass. A slightly different fitting strategy consists of simultaneously fitting the two- and three-point function for each jackknife data set. This method has the added advantage that the above mentioned correlations between the two Green's functions are taken into account. Afterwards, a check should be made to see if the excited state parameters, which are also influenced by the three-point function, agree with the ones obtained from a single fit to the two-point function.

Deciding between the two fit methods as outlined above, we favour the simultaneous

**Figure 5.2:** Examples of three-point functions for different parameters.
5.4. Analysis methods

fit, since it takes into account the correlations. Our fit parameters will be the ground and excited state energies and amplitudes $Z$, the form factor and the pre-factors of the transition terms. These last two parameters are a combination of the transition form factors and the corresponding $Z$-factors. We choose to combine them since it makes the fit more stable and we are not interested in the extraction of these transition form factors. The excited state energy and amplitude are assumed to be $Q^2$-independent, but were separately fitted for each $Q^2$ for convenience. We will comment on this in Sec. 5.5.

In the case of the conserved current, the time interval $[0 : 10]$ is used for the fit, only excluding the last time slice ($t = 11$)\(^1\). The source ($t = 0$) does not coincide with the first photon insertion 'point' since the current is divided over two time slices. Because of this structure of the conserved current, confusion might arise about the time slice on which the current is defined. To avoid this, one can construct the symmetric version of the conserved current \([10,23]\),

$$ j_{\mu}^{C,\text{symm}}(x) = \frac{1}{2} \left( j_{\mu}^{C}(x) + j_{\mu}^{C}(x - \hat{\mu}) \right). \quad (5.23) $$

The fit interval reduces to $[1 : 10]$ but the results are unchanged. We therefore simply use the non-symmetrised version of this current. To avoid contact terms in case of the (renormalised) local and improved currents the fit interval is chosen to be $[1 : 10]$.

As discussed above, the transition contributions are included in our parametrisation to better describe the data. Since we use the complete time interval of the three-point function, the state with $n = 1$ does not necessarily represent a genuine single excited state, rather it parametrises contributions from all possible excited states. We want the same combination of excited states to contribute in the two-point function in order to keep the definition of our effective excited state the same. In the fit of the two-point function, one therefore has to include the data points closest to the source and sink.

A comparison between the simultaneous fit and the ratio method will be made in Sec. 5.5.

5.4.1. $Q^2 = 0$: the second insertion test

In the forward direction, \textit{i.e.} for $Q^2 = 0$, we have a different method to obtain the form factor. By exploiting current conservation, we can relate two contributions of the time-ordered three-point function to the pion propagator (see Sec. 5.2.1).

For the case of the conserved current, this procedure is readily applicable. The ratio of the l.h.s. and r.h.s of Eq. 5.20 is calculated per configuration and should yield 1 to within a certain precision as first demonstrated by [10]. Deviations only show up due to the numerical approximation while current conservation prevents fluctuations originating from physical effects.

\(^1\)From the structure of the conserved current, Eq. 3.33, one sees that the last data point is actually the first time slice of the second insertion.
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From Fig. 5.2(c) we see that for $Q^2 = 0$, the conserved current is constant in $t$ to high precision. This can be expected, since the transition form factors vanish for $Q^2 = 0$. The numerical data confirm this picture: the conserved current is constant within fluctuations of $\mathcal{O}(10^{-5})$. The only possible contribution from excited states originates from elastic excited state interactions. We see that the ratio of the three- and two-point Green’s functions, as calculated from Eq. 5.20, reduces to $F(0)$, regardless of how many excited states are present. We thus do not need to assume that the elastic excited state contribution is small.

The second insertion, with $t_f < t$ (not shown), displays the same constant behaviour. Therefore, we do not need to compute the second insertion for the complete time range. We have used only one time slice beyond $t_f$ and found $F(0) = 1$ with fluctuations of only $\mathcal{O}(10^{-5})$ for each configuration separately.

Two configurations showed a time dependence for $Q^2 = 0$, and (consequently) their value for $F(0) \neq 1$. These configurations were regarded as exceptional and left out of the data sample. Closer inspection showed that the pion mass for these configurations was substantially larger than normal. Also, the inversion of the fermion matrix for the highest $\kappa$-value (lowest mass) failed to converge for these configurations.

The case of the renormalised local current is a little more involved, since the current is not conserved but only renormalised. The two- and three-point correlation functions are therefore not ‘protected’ by Eq. 5.20, i.e. fluctuations in the ratio can be due to physical effects, and their ratio on a single configuration need not be 1. We therefore turn to jackknife sets to calculate the average ratio. Since the three-point function for $Q^2 = 0$ is not constant in this case, (see Fig. 5.2(a)), we cannot be convinced that transition matrix elements are actually absent (although they should). Since the onset of a plateau is however visible, we calculate the ratio for decreasing time ranges and look for stability. In case the time dependence of the three-point function is a real effect, we choose the second insertion in such a way that these effects are expected to be equally present in both contributions. We calculate the second insertion for 10 time slices beyond $t_f$ for a subset of approximately 20 configurations. The l.h.s. of Eq. 5.20 is averaged over pairs of values $t$ and $t'$ symmetric around $t_f$ and normalised by the 2-point function. A jackknife analysis on the subset is performed and a range of 4-6 time slices is chosen. Using the renormalisation constants as determined by Bhattacharya et al. [62], we obtain $F(0) = F_{RL}(0) \approx 1$, with an error of 0.2-2%, depending on the pion mass. This procedure yields a much more precise result than we would have obtained from simply taking the ratio, although not as precise as the results for the conserved current.

Instead of using the $Z_V$ factor from [62] to renormalise the local current, we can also define a (mass-dependent) renormalisation factor by demanding

$$R^L_{RL} = Z_V C_{4,3}(t_f, t; \mathbf{p}, \mathbf{p}, 0)/G^{(2)}(t_f; \mathbf{p}) \equiv 1$$  \hspace{1cm} (5.24)$$

for the three-point function based on the local current. The results for the $Z_V$-values are

---

2The renormalised local current is identical to the improved current for forward matrix elements.
Table 5.1: Extracted values for the renormalisation constants; (a) mass-dependent (b) mass-independent

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<th>$m_\pi$</th>
<th>$R^L$</th>
<th>$Z_V$ (this work)</th>
<th>$Z_V$ from [62]</th>
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<td>0.516</td>
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<td>0.875(3)</td>
<td>0.868(1)</td>
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<td>$Z_V^0$</td>
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<td>0.770(1)</td>
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<tr>
<td>$b_V$</td>
<td>1.53(8)</td>
<td>1.52(1)</td>
</tr>
</tbody>
</table>

5.5. Systematic uncertainties

As stated before, other collaborations, which used Dirichlet boundary conditions, have chosen to use ratio’s of three- and two-point function to extract the form factor from the data. However, the ratio method only produces an accurate estimate of the form factor if excited states have died out sufficiently. In order to take into account these excited states, we proposed to use simultaneous fits. In this section, we will discuss both methods and investigate their systematic errors. The methods are then compared for our heaviest and lightest pion.

To determine the ratio, consider the parameterisations, Eq. 4.4 for the two-point- and 5.10 for the three-point function. In the last parametrisation, we only take into account the elastic form factor(s). Together with our choice for initial and final momenta
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$(p_r^2 = p_t^2)$, the ratio is seen to approximately reduce to the form factor

$$\frac{\tilde{G}_{A,R}(t_f, t; p_f, q)}{\tilde{G}_{R}(t_f, 0; p_f)} \to F(Q^2).$$  (5.26)

Aside from the systematic uncertainties to be discussed below, there is a principal problem for our periodic boundary conditions. Even in the absence of an excited state contribution, the ratio yields the form factor only approximately. This is because the total charge, as probed by the current insertion, is not exactly equal to 1 when the second insertion is not included. Since we only obtained data for the second insertion on a subset of the available configurations, it is not feasible to try and include this contribution in the determination of the ratio. In Sec. 5.2 the contribution was estimated and considered negligible. Based on the operator insertion times and the energies for a pion with momentum $p^2 = 0.137$, we estimate the relative contribution to be approximately $0.1 - 0.9\%$. If the two methods would be equally good, there will still be a difference of this size, due to our boundary conditions.

The ratio is taken using the jackknife sets and the 'plateau' is fitted for decreasing fit range until stability is found. The first thing to note is that the data does not always reach an asymptotic value. To illustrate this point, data for two fit ranges (two and four) have been calculated.

To compare the results of both methods, we also investigate the potential systematic errors of the simultaneous fit method. A possible source of these systematic uncertainties is a wrong parametrisation of the excited states.

As a first test, we performed the simultaneous fit excluding a pair of data points closest to the source and sink in both the two- and three-point function. In this way we change the contribution of our excited state equally in both correlation functions. If our parameterisations and assumptions are correct, this procedure should yield the same results for the form factor. We indeed find similar results. Upon reducing the fit range, the form factor increases slightly, notably for the higher $Q^2$-values. This amounts (upon averaging) to results that are spread around the central value with a sigma of 0.02 ($\approx 8\%$) for the highest $\kappa$-value. This reduction of the fit range could change the error on the form factor, because the fit range becomes smaller, but we observed no significant change in the $\chi^2$/d.o.f of the fit. An increase of the error bars on the excited state parameters, however, was observed for the smaller fit range. When reducing the fit range with only a pair of time slices, these errors have already increased with 10-15%. A further reduction of the fit range is therefore not reasonable, since the determination of the contribution from the 'excited state' becomes so inaccurate that a sensible extraction of the form factor is not possible. We therefore choose to average the results for the two fits and include the systematic uncertainty in the errors.

Secondly, in Sec. 5.4, we stated that we have to ensure that the fitted excited state parametrises the contributions from the same combination of excited states in both the two- and three-point function. We will test this below by comparing the simultaneous fit parameters with the results of the fit to the two-point function only.
### Table 5.2: Excited state energies obtained from the simultaneous fit. Last row: values from the two-point function alone.

<table>
<thead>
<tr>
<th>$Q^2 \backslash m_{\pi}$</th>
<th>0.516</th>
<th>0.414</th>
<th>0.356</th>
<th>0.287</th>
<th>0.194</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.137</td>
<td>1.021(28)</td>
<td>0.993(36)</td>
<td>0.978(48)</td>
<td>0.99(10)</td>
<td>0.97(13)</td>
</tr>
<tr>
<td>0.274</td>
<td>1.021(27)</td>
<td>0.993(36)</td>
<td>0.978(47)</td>
<td>1.00(10)</td>
<td>0.98(14)</td>
</tr>
<tr>
<td>0.411</td>
<td>1.007(36)</td>
<td>0.992(35)</td>
<td>0.946(66)</td>
<td>0.92(9)</td>
<td>0.98(14)</td>
</tr>
<tr>
<td>0.548</td>
<td>1.021(28)</td>
<td>0.992(36)</td>
<td>0.977(48)</td>
<td>0.99(10)</td>
<td>0.98(14)</td>
</tr>
<tr>
<td>2-p. res.</td>
<td>1.022(28)</td>
<td>0.993(36)</td>
<td>0.969(40)</td>
<td>0.99(10)</td>
<td>0.98(14)</td>
</tr>
</tbody>
</table>

However, the parameters in the simultaneous fit are to a large extent determined by the two-point function and the excited state amplitudes are not fitted separately in the simultaneous fit. Therefore, the only parameter which appears in the parametrisation of both functions, and can be influenced by the three-point function, is the excited state energy. We thus need to check if this parameter is the same in both fits.

Thirdly, in principle, an admixture of genuine transition form factors $0 \leftrightarrow 1$, $0 \leftrightarrow 2$ and possible even higher states, which might have different $Q^2$ dependencies could introduce some $Q^2$ dependence into the effective fit parameter, $E_1$. Whether this is the case, can also easily be checked by the studying the excited state energy in more detail. Our excited state energies as obtained from the simultaneous fits, compared to the ones from the fits to the two-point function, are shown in Table 5.2 for different $Q^2$ and largest fit range. We observe that the fitted excited state in both fits are equal to high accuracy. This means that both fits parametrise the same combination of true excited states into one effective state\(^3\). A further observation is that the data shows no indication of a $Q^2$-dependence of the 'excited state' energy. The ansatz of a $Q^2$-independent excited state is thus permitted.

The results of both extraction methods for the two masses are given in Table 5.3. The ratio method is seen to yield results which have smaller errors by a factor of 2 for the highest mass. This is not surprising, since correlations are better taken into account when taking a ratio.

For the lightest pion, the two methods have similar errors. The results from the ratio method are systematically larger than those from the simultaneous fits. It is also seen that this difference increases with increasing $Q^2$ and decreasing pion mass. Since this trend is seen for every pion mass, we conclude that it is a systematic difference between the two methods, even though the error bars cover the gap in case of the lighter quarks.

From the numerical results alone, one cannot simply favour one method over the other. However, for the ratio method one assumes that the excited states have died

\(^3\)Note that in Table 5.2, the data for $Q^2 = 0.411$ and pion masses 0.516, 0.356 and 0.287, is extracted using less configurations (approximately 50). This is the reason for the slight deviation from the results for the other $Q^2$ values. In the fitting procedure, this fact was taken into account by evaluating the two-point function on the same reduced set of configurations.
Chapter 5. Analysis of the three-point function: extraction of the form factor at $T = 0$

Table 5.3: Comparison of the two analysis methods for (a) $m_\pi = 0.516$ and (b) $m_\pi = 0.194$.

<table>
<thead>
<tr>
<th>$Q^2$</th>
<th>Ratio method</th>
<th>Sim. fit</th>
<th>Ratio method</th>
<th>Sim. fit</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.137</td>
<td>0.738(10)</td>
<td>0.736(10)</td>
<td>0.717(24)</td>
<td></td>
</tr>
<tr>
<td>0.274</td>
<td>0.606(12)</td>
<td>0.602(12)</td>
<td>0.563(20)</td>
<td></td>
</tr>
<tr>
<td>0.411</td>
<td>0.490(10)</td>
<td>0.485(10)</td>
<td>0.429(23)</td>
<td></td>
</tr>
<tr>
<td>0.548</td>
<td>0.419(9)</td>
<td>0.413(10)</td>
<td>0.347(22)</td>
<td></td>
</tr>
</tbody>
</table>

(a)  

out. This is unlikely, even for the middle time slices, as can be seen from Fig. 5.2, and leads to a systematic uncertainty, which is a priori unknown. Since we have better understanding and control over the systematic uncertainties in case of the simultaneous fit method, we prefer this method and use it in our subsequent analysis.

5.6. Comparison of the currents

In Sec. 3.5, we have discussed various forms of the lattice vector current. In this section we will discuss the results obtained with the different currents. In order to extract the form factor we will use the simultaneous fit method as described in Sec. 5.4, complemented with the averaging of the results from two fit ranges, as discussed in Sec. 5.5, to correct for the systematic errors.

The results for the different currents are summarised in Table 5.4 and, for two of our pion masses, displayed in Fig. 5.3. Similar figures for the other three pion masses can be found in App. A.2.

First of all, we see that the results are more accurate for heavier pions. But even for the lightest pion, although with large error bars, a rather smooth $Q^2$-dependence of the form factor can still be seen. We observe that the difference between conserved and improved current increases with momentum transfer and decreasing mass, indicating a substantial $O(a)$ correction. The differences between the improved and renormalised local current are due to the tensor term. Although this contribution increases with $Q^2$, the improved form factor stays very close to the result for the renormalised local current, even for the lightest pion and up to the largest momentum transfer considered in this work. This indicates that the contribution of the tensor term in the improved current is small. While the matrix element of this tensor operator can become comparable in size (up to 70%) to the local current operator, its contribution to the form factor is small since the improvement coefficient we use, $c_V = -0.107$, determined in [62].
5.6. Comparison of the currents

Table 5.4: Form factor extracted from different currents for several masses.

<table>
<thead>
<tr>
<th>$Q^2$</th>
<th>$j_4^l$</th>
<th>$j_4^C$</th>
<th>$j_4^L$</th>
<th>$j_4^l$</th>
<th>$j_4^C$</th>
<th>$j_4^L$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.992(3)</td>
<td>1.00000(1)</td>
<td>0.992(3)</td>
<td>0.993(2)</td>
<td>1.00000(1)</td>
<td>0.993(2)</td>
</tr>
<tr>
<td>0.137</td>
<td>0.717(24)</td>
<td>0.765(24)</td>
<td>0.705(24)</td>
<td>0.670(28)</td>
<td>0.719(29)</td>
<td>0.658(28)</td>
</tr>
<tr>
<td>0.274</td>
<td>0.563(20)</td>
<td>0.635(22)</td>
<td>0.546(19)</td>
<td>0.514(22)</td>
<td>0.587(24)</td>
<td>0.498(22)</td>
</tr>
<tr>
<td>0.411</td>
<td>0.429(23)</td>
<td>0.511(27)</td>
<td>0.409(26)</td>
<td>0.380(20)</td>
<td>0.463(22)</td>
<td>0.360(19)</td>
</tr>
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<td>0.548</td>
<td>0.347(22)</td>
<td>0.434(26)</td>
<td>0.326(22)</td>
<td>0.307(26)</td>
<td>0.394(29)</td>
<td>0.287(25)</td>
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</tbody>
</table>

(a) $m_\pi = 0.516$.

<table>
<thead>
<tr>
<th>$Q^2$</th>
<th>$j_4^l$</th>
<th>$j_4^C$</th>
<th>$j_4^L$</th>
<th>$j_4^l$</th>
<th>$j_4^C$</th>
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<td>1.00000(1)</td>
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<td>0.639(32)</td>
<td>0.689(32)</td>
<td>0.628(31)</td>
<td>0.615(37)</td>
<td>0.665(38)</td>
<td>0.604(37)</td>
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<td>0.274</td>
<td>0.486(26)</td>
<td>0.558(26)</td>
<td>0.470(25)</td>
<td>0.460(31)</td>
<td>0.529(32)</td>
<td>0.445(30)</td>
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<tr>
<td>0.411</td>
<td>0.370(29)</td>
<td>0.451(33)</td>
<td>0.351(28)</td>
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<td>0.264(31)</td>
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<td>0.345(47)</td>
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(b) $m_\pi = 0.414$.

<table>
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<th>$Q^2$</th>
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<th>$j_4^l$</th>
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<td>0.665(38)</td>
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<td>0.425(70)</td>
<td>0.487(76)</td>
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<td>0.529(32)</td>
<td>0.445(30)</td>
</tr>
<tr>
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<td>0.423(89)</td>
<td>0.295(69)</td>
<td>0.356(36)</td>
<td>0.435(44)</td>
<td>0.338(3)</td>
</tr>
<tr>
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<td>0.32(13)</td>
<td>0.216(99)</td>
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<td>0.345(47)</td>
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(c) $m_\pi = 0.356$.

<table>
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<td>0.601(72)</td>
<td>0.615(37)</td>
<td>0.665(38)</td>
<td>0.604(37)</td>
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<td>0.412(71)</td>
<td>0.460(31)</td>
<td>0.529(32)</td>
<td>0.445(30)</td>
</tr>
<tr>
<td>0.411</td>
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<td>0.423(89)</td>
<td>0.295(69)</td>
<td>0.356(36)</td>
<td>0.435(44)</td>
<td>0.338(3)</td>
</tr>
<tr>
<td>0.548</td>
<td>0.236(99)</td>
<td>0.32(13)</td>
<td>0.216(99)</td>
<td>0.259(41)</td>
<td>0.345(47)</td>
<td>0.240(41)</td>
</tr>
</tbody>
</table>

(d) $m_\pi = 0.287$.

<table>
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<tr>
<th>$Q^2$</th>
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<th>$j_4^C$</th>
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<th>$j_4^l$</th>
<th>$j_4^C$</th>
<th>$j_4^L$</th>
</tr>
</thead>
<tbody>
<tr>
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<td>1.00(2)</td>
<td>0.993(2)</td>
<td>1.00000(1)</td>
<td>0.993(2)</td>
</tr>
<tr>
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<td>0.664(78)</td>
<td>0.601(72)</td>
<td>0.615(37)</td>
<td>0.665(38)</td>
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<td>0.412(71)</td>
<td>0.460(31)</td>
<td>0.529(32)</td>
<td>0.445(30)</td>
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<td>0.423(89)</td>
<td>0.295(69)</td>
<td>0.356(36)</td>
<td>0.435(44)</td>
<td>0.338(3)</td>
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<td>0.32(13)</td>
<td>0.216(99)</td>
<td>0.259(41)</td>
<td>0.345(47)</td>
<td>0.240(41)</td>
</tr>
</tbody>
</table>

(e) $m_\pi = 0.194$.

is rather small. The preliminary value obtained by the ALPHA collaboration [75] is larger, $c_V = -0.32$. Since the improved current is a linear combination of the local and the tensor term, Eq. 3.36, the change in the improved current due to a change in $c_V$ is straightforward. The difference between the two values of $c_V$ is of order $a$, resulting in improved currents which are different at $\mathcal{O}(a^2)$. Using our results, we find that $\mathcal{O}(a^2)$ effects can still become as large as 10 % at higher momentum transfers and low masses.
Chapter 5. Analysis of the three-point function: extraction of the form factor at $T = 0$

Figure 5.3: Form factors extracted for different currents as a function of $Q^2$ for two pion masses. Solid curves: VMD prediction with $m_Y = m_\rho$ taken from [65] at the $\kappa$-values.

The curves are predictions based on the Vector Meson Dominance ansatz, which will be discussed in more detail in the next section.
5.7. The form factor and vector meson dominance

A quite successful model for describing the experimental data as well as early lattice calculations [10], is the so-called Vector Meson Dominance (VMD) model. This model is based on an effective field theory, in which the photon can fluctuate into a vector meson before coupling to the pion. For our purposes, i.e. in the space-like regime and for relatively small momentum transfers, it suffices to consider a rho meson. Features like e.g. rho-omega mixing only become important in the time-like regime in the vicinity of the rho resonance. For the form factor, this idea is schematically depicted in Fig. 5.4. There actually exist different versions of the VMD model; see [76] for a review. Two versions were first discussed by Sakurai [77]; the underlying Lagrangians differ in the way they treat the interaction of the photon with hadronic matter. The first version, in which the photon is allowed to couple to both the pion and the rho-meson, yields the following expression for the form factor

\[ F(Q^2) = 1 - \frac{Q^2}{m_\rho^2 + Q^2} g_{\rho\pi\pi} \]

where \( g_{\rho\pi\pi} \) is the coupling of the \( \rho \)-meson to the pions and \( g_\rho \) determines the coupling of the \( \rho \) to the photon. The well-known constraint \( F(0) = 1 \), is automatically satisfied. In the second, and more popular version of VMD, the Lagrangian only includes a coupling of the photon to the rho. In this second case, the form factor can be written as

\[ F(Q^2) = \frac{m_\rho^2}{m_\rho^2 + Q^2} g_{\rho\pi\pi} / g_\rho. \]

Here, the constraint \( F(0) = 1 \) is not automatically satisfied and we need to enforce universality, i.e. we need to demand \( g_{\rho\pi\pi} = g_\rho \). This can alternatively be viewed as a consequence that in the second version the vector dominance is total, i.e. there is no direct coupling of the photon to the pions. Note that in both models the interactions are point-like and therefore assume that there is no momentum dependence of the coupling constants. In the limit of universality, both versions are identical.
Chapter 5. Analysis of the three-point function: extraction of the form factor at $T = 0$

Table 5.5: Results from fits to the two VMD inspired descriptions of the form factor.

<table>
<thead>
<tr>
<th></th>
<th>From [65].</th>
<th>VMD (Eq. 5.27)</th>
<th>VMD (Eq. 5.29)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m_\pi$</td>
<td>$m_\rho$</td>
<td>$m_V$</td>
<td>$g_{V\pi\pi}/g_V$</td>
</tr>
<tr>
<td>0.516</td>
<td>0.623(2)</td>
<td>0.68(13)</td>
<td>1.21(27)</td>
</tr>
<tr>
<td>0.414</td>
<td>0.550(2)</td>
<td>0.60(10)</td>
<td>1.16(21)</td>
</tr>
<tr>
<td>0.356</td>
<td>0.515(3)</td>
<td>0.51(9)</td>
<td>1.01(18)</td>
</tr>
<tr>
<td>0.287</td>
<td>0.485(3)</td>
<td>0.46(9)</td>
<td>0.97(17)</td>
</tr>
<tr>
<td>0.194</td>
<td>0.448(13)</td>
<td>0.50(20)</td>
<td>1.10(40)</td>
</tr>
</tbody>
</table>

In Fig. 5.3, we already showed VMD curves with $m_\rho$, the lattice $\rho$-mass calculated at the same $\kappa$-value (quark mass) [65] and assuming universality. At large pion mass the VMD-prediction describes the form factor based on the conserved current reasonably well but lies systematically above the results for the more accurate improved current. However, at lower pion masses, the model prediction shifts toward the improved form factor results.

To investigate this point in more detail we fitted our improved form factors, using a general vector meson mass, $m_V$, as the fit parameter. In the first fit, we use the version without universality, Eq. 5.27. In principle, more than one vector meson could contribute, but taking into account these heavier vector mesons, as suggested by some extended VMD models [78], is not feasible, since it would introduce too many fit parameters and therefore destabilise the fit. Since the model is meant to apply at moderate $Q^2$ ($\leq 1$ GeV$^2$), we exclude the highest $Q^2$ point in the fit and extract the parameters. We then exclude one more data point and observe that the parameters are not stable under this reduction. This might indicate that $Q^2 = 0.411$ is still too high. A more plausible explanation is that the number of d.o.f. of the fit is already too small upon leaving out one data point, since a further reduction leads to a fit with zero d.o.f.

In Table 5.5 we therefore show, for illustration purposes only, the results of the fit in which only the highest $Q^2$ has been left out. We first of all observe that the error bars are large, especially in comparison to the fit to Eq. 5.29 (see discussion below). Furthermore, the extracted ratio of couplings depends non-trivially on the quark mass, although it agrees, within the large error bars, with the experimentally observed value, $g_{\rho\pi\pi}/g_\rho = 1.22(2)$ [78]. The vector meson mass which we extract fluctuates around the rho mass, but the difference is seen to decrease with the quark mass, although the results for the lightest pion mass are disputable. These considerations lead us to believe that the data is not accurate and stable enough for a fit to Eq. 5.27 to give sensible results.
5.7. The form factor and vector meson dominance

Figure 5.5: Form factor extracted from the improved current as a function of $Q^2$ for different $m_\pi$. Curves: fits to the VMD-model, Eq. 5.29.

Alternatively, we assume universality and use the simple monopole form

$$F(Q^2) = \frac{1}{1 + Q^2/m_v^2}. \quad (5.29)$$

We again excluded the highest $Q^2$ point and fit the data to obtain the 'mass' parameter $m_V$. A second fit, in which a additional $Q^2$ point was excluded, yielded similar results. Since we have no argument to favour one of the two fits, we simply average them. The results for the vector meson mass from this method are also displayed in Table 5.5. We see that the vector meson mass decreases with the quark mass, as expected. Furthermore, the results are more accurate than those obtained with the fit to Eq. 5.27. The vector meson mass as extracted from the fits is seen to come closer to the lattice $\rho$-mass for decreasing quark mass. This might indicate that this VMD-model describes the form factor better in the physical limit. However, we will see in Sec. 5.9 that the experimental data is accurately described by the simple monopole form of Eq.5.29, with $m_V \neq m_\rho$.

We show the improved currents as a function of $Q^2$ for our five different masses in Fig. 5.5. The curves are fits to the model, Eq. 5.29, in which we have excluded the highest $Q^2$-point(s). From the figure, we see that the simple monopole parametrisation with unspecified vector meson mass, is quite successful in describing the lattice data for low $Q^2$. Therefore, this parametrisation can be used in the determination of the charge radius of the pion, as we will do in the Sec. 5.10.
5.8. Determination of the scale

In order to compare our results to the experimental data, we need to set the scale of the lattice calculations. We will only shortly discuss the methods used. The scale can be set using different observables, such as the \( \rho \)-mass or the string tension. Klassen et al. [61] used the latter to set the scale. They calculated the string tension for several couplings in the pure gauge sector, complemented their data set with lattice results available in the literature and fitted all data as a function of \( g^2 \). With their phenomenological fit, it is then possible to obtain the string tension at any given value of the coupling \( g^2 \). Comparing with the physical value then gives an estimate for the lattice spacing. This physical value of the string tension, however, is not known to high accuracy. The authors of [61] use a relatively high estimate, \( \sqrt{\sigma} = 465 \text{ MeV} \). For definiteness we have chosen to use the average value of \( \sqrt{\sigma} = 420 \text{ MeV} \). With that choice we find \( a = 0.105 \text{ fm} = (1.91 \text{ GeV}^{-1}) \). This value is in agreement with other estimates e.g. [79], where the authors use the \( \rho \)-mass to set the scale. The different determinations of the scale can differ by 10 %, but agree within the error bars. These differences depend strongly on the observable used. The uncertainty in the scale should be kept in mind when we present our results in physical units.

5.9. Comparison to experiment

In Fig. 5.6, we show our results together with the available measurements [80, 81]. For clarity, we only show our results for three \( \kappa \)-values. As can be clearly seen, our calculated form factors, regardless of the mass, lie above the experimental values. A continuous trend toward the measured values for decreasing mass can be observed. Although our lightest pion mass is still more than twice as heavy as the physical pion, we come rather close to the measurements. Whether a further straightforward lowering of the pion mass alone will resolve the remaining discrepancy between our calculations and experiment, is not clear.

The solid line in the figure shows the monopole form, Eq. 5.29, based on a fit to the experimental data with \( Q^2 \leq 1.5 \text{ GeV}^2 \). We find \( m_V = 690 \text{ MeV} \). Using only the data points with \( Q^2 \leq 1.0 \text{ GeV}^2 \), we find \( m_V = 721 \text{ MeV} \). Both masses are significantly lower than the experimental value for the \( \rho \)-mass \( (m_\rho = 770 \text{ MeV}) \), emphasising that the VMD-inspired monopole description provides a successful parametrisation of the form factor data, but does not hold in detail.

5.10. The pion charge radius

It is well known that the form factor can be related to the charge radius of the pion. To see this, recall that in quantum mechanics, the form factor can be written as the
Figure 5.6: The form factor for different $m_\pi$, compared to experiment [80,81]

Fourier transform of the normalised charge distribution $\rho(x)$

$$F(q) = \int \frac{d^3 x}{(2\pi)^3} e^{i q \cdot x} \rho(x).$$  \hfill (5.30)

If we assume spherical symmetry and expand the exponential, we obtain

$$F(|q|) = 1 - \frac{1}{6} \langle r^2 \rangle |q|^2 + \mathcal{O}(|q|^4).$$  \hfill (5.31)

From this we see that the root mean square (RMS) radius of the pion can be written as:

$$\langle r^2 \rangle = 6 \left. \frac{\partial F(Q^2)}{\partial Q^2} \right|_{Q^2=0}$$  \hfill (5.32)

where we have gone back to our usual notation with $Q^2 = -q^2$. In contrast to the charge-radius extracted from the Bethe-Salpeter amplitude, this determination of $\langle r^2 \rangle$ is not based on any specific assumptions about the motion of the quarks and gluons inside the pion. Since the vector meson model works very well as a parametrisation of our results for low $Q^2$, we simply calculate the mean square radius of the pion obtained
Chapter 5. Analysis of the three-point function: extraction of the form factor at \( T = 0 \)

### Table 5.6: Pion radii from the form factor, compared to the BS results.

<table>
<thead>
<tr>
<th>( m_\pi )</th>
<th>( \langle r^2 \rangle_{FF} )</th>
<th>( \langle r^2 \rangle_{BS} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.516</td>
<td>17.4(11)</td>
<td>12.78(4)</td>
</tr>
<tr>
<td>0.414</td>
<td>21.5(14)</td>
<td>13.38(6)</td>
</tr>
<tr>
<td>0.356</td>
<td>23.9(18)</td>
<td>13.62(6)</td>
</tr>
<tr>
<td>0.287</td>
<td>26.4(23)</td>
<td>13.83(4)</td>
</tr>
<tr>
<td>0.194</td>
<td>29.1(55)</td>
<td>13.83(7)</td>
</tr>
</tbody>
</table>

From the monopole form, Eq. 5.29, which yields

\[
\langle r^2 \rangle = \frac{6}{m_\pi^2}. \tag{5.33}
\]

In the following, we only show results based on the improved current. By looking at Table 5.6, we observe that the \( \langle r^2 \rangle \) thus obtained shows a considerable mass dependence. This is in contrast to the BS results from Chapter 4, which are repeated for convenience. Moreover, the form factor based results are significantly larger than the BS results. As discussed by Gupta et. al. [52], this can be due to how one treats the centre-of-mass of the two quarks. For example, the influence of gluons on this centre-of-mass is not considered in the BS approach. However, as these authors also point out, the value extracted through the form factor contains a contribution which is absent when calculating the \( \langle r^2 \rangle \) from the Bethe-Salpeter amplitudes. The corresponding diagram is depicted in Fig. 5.7. It essentially describes the screening of the strong force through the formation of a quark-anti-quark pair [52]. In principle, such diagrams are also present in the two point function, but the Bethe-Salpeter amplitudes are insensitive to them since they 'measure' only the quark-anti-quark state. This screening of the colour charge, however, can lead to an enlargement of the electro-magnetic charge radius of the pion [52].

The \( \langle r^2 \rangle \) values obtained from the form factor (using \( a = 0.105 \) fm) can be seen to get closer to the physical value of \( \langle r^2 \rangle = 0.439(8) \) fm\(^2\) [74] as the pion mass decreases. This encourages us to try several extrapolations to the physical limit which will be described in the next section.

#### 5.10.1. Extrapolation in \( m_\pi \)

To obtain physical results, one can try to extrapolate in the pion mass. We take \( \langle r^2 \rangle \) as the quantity to extrapolate since it is also known experimentally and there is theoretical guidance for the extrapolation in the pion mass. We consider three
types of extrapolations. From chiral perturbation theory $\chi PT$, one knows the one-loop result [82],

$$\langle r^2 \rangle^\text{one-loop}_{\chi PT} = c_1 + c_2 \ln m_\pi^2$$  \hspace{1cm} (5.34)

In our fit, we will treat $c_1$ and $c_2$ as free parameters. In quenched $\chi PT$, the radius is constant at this order of expansion [83]. It is, however, expected that this situation will change at the two-loop level, which will introduce terms like

$$\langle r^2 \rangle^\text{two-loop}_{q\chi PT} = d_1 \frac{1}{m_\pi^2} + d_2 \ln m_\pi^2 + d_3 m_\pi^2$$  \hspace{1cm} (5.35)

including a term linear in $m_\pi^2$ which, for our pion masses, can be expected to yield the dominant contribution [83, 84]. We therefore only tried to fit a form containing a constant plus a linear term in $m_\pi^2$.

We have observed in Sec. 5.7 that the form factor data could be well parametrised by a simple monopole form as suggested by vector meson dominance. We use this finding to construct an additional extrapolation. Since it can be seen from Table 5.5 that the fitted parameter, $m_V$ (like $m_\rho$), scales approximately linear with $m_\pi^2$, one can use Eq. 5.33 to parametrise the radius as

$$\langle r^2 \rangle_{\text{VMD}} = \frac{6}{b_1 + b_2 m_\pi^2}.$$  \hspace{1cm} (5.36)

The results for $\langle r^2 \rangle$, together with the three extrapolations, are plotted in Fig. 5.8. The extrapolated value for the radius is seen to depend strongly on the method chosen. The VMD ansatz describes our data best. If we use this prescription to extrapolate to the physical pion mass, we find

$$\langle r^2 \rangle = 0.36(2) \text{ fm}^2,$$  \hspace{1cm} (5.37)

which lies below the experimental value $\langle r^2 \rangle = 0.439(8) \text{ fm}^2$. This could clearly be due to the extrapolation chosen, but also due to approximations, such as quenching, inherent in our approach.

5.11. Conclusions

We have presented calculations for the pion form factor that improved and extended previous work in several respects. First, we have pushed the form factor calculations for a large range of $Q^2$ toward much lower pion masses than the earlier calculation at $m_\pi \approx 1 \text{ GeV}$. Secondly, we have worked in a framework that guarantees the absence of $O(a)$ corrections. This meant a consistent use of an improved action together with the concomitant improved current. We have shown that use of this current leads to significant changes over results based on the conserved Noether current for this action, which still contains $O(a)$ corrections at finite $Q^2$. An important element in our
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![Graph](image)

**Figure 5.8: Extrapolation of $\langle r^2 \rangle$**

The calculation is to choose the kinematics in such a way that the initial and final pion three-momentum have the same absolute value. This leads to considerable simplifications when extracting the form factor.

Our results for the form factor were seen to smoothly decrease with the pion mass. The lower $Q^2$ results could all be described quite well by a simple monopole form factor. The fitted range parameter $m_V^{-1}$ was, for each $\kappa$-value, found to be close to the corresponding lattice $\rho$-mass. The agreement between the two values got closer for decreasing pion mass, indicating better agreement with the prediction from the vector meson dominance model.

When compared to the experimental form factor, it could be seen that our results consistently approach the data from above over the entire range of $Q^2$-values we consider. While gauge invariance fixes all form factors in the forward direction, $F(0) = 1$, we found that the calculated form factor at $Q^2 > 0$ comes close to the experimentally determined shape. This shows that by means of lattice methods, QCD indeed is able to describe a purely non-perturbative feature such as the pion form factor quite realistically and in detail from first principles. However, a straightforward extension of our approach to even lower pion masses is not necessarily the way to proceed to close the last gap with the experiment. Improvements of our methods and the use of new lattice
techniques will become increasingly important, *e.g.* one has to understand the rôle of dynamical quarks, which are neglected in the quenched approximation.

The form factor can be used to reliably extract the mean square charge radius of the pion. We showed that the estimates for \( \langle r^2 \rangle \) based on the Bethe-Salpeter amplitudes of the previous chapter are qualitatively as well as quantitatively not very reliable. Disagreement up to a factor of two was found with the form factor based values. Furthermore, these values showed quite a pronounced mass dependence in contrast to the BS results. Extrapolations of our charge radii toward the physical pion mass were shown to lead to no unique prediction. The best description of the results at our pion masses was provided by a vector meson dominance inspired model. When extrapolated to the physical pion mass, it yielded a value for \( \langle r^2 \rangle \) about 15% below the experimental value. For an extrapolation inspired by (quenched) chiral perturbation theory our pion masses are not low enough to be sufficiently sensitive to the predicted \( \ln m_\pi^2 \) terms.

As is well known, Wilson fermions have the major disadvantage that chiral symmetry is broken, in order to remove the doublers, resulting in errors already at \( \mathcal{O}(a) \). This was one of the reasons improvement was invented and why we chose a framework where the action and operators where consistently improved such that only corrections to \( \mathcal{O}(a^2) \) occur.

Another method, among others, is the introduction of a fifth dimension and the use of so-called domain wall fermions. Chiral symmetry is then not tied to taking the continuum limit. The price one pays is a substantial increase in computer time. The RBC collaboration has chosen this approach and first results can be found in [85]. In this paper, pion masses down to 390 MeV are used, albeit on a coarser lattice. Their results obtained so far at two low \( Q^2 \) points, based on the renormalised local current, seem to agree reasonably well with our values. Differences with our implementation of chiral symmetry show up at \( \mathcal{O}(a^2) \).

In our work we have assumed, as is often done, that the quenched approximation can be used. The influence it has on our observables is largely unknown. Although it is beyond the scope of this thesis to investigate the form factor using dynamical quarks, some remarks can be made. Alexandrou *et al.* [86] have calculated density-density correlations for the \( \pi, \rho, N \) and \( \Delta \) in quenched as well as in full QCD. In contrast to the \( \rho \) and \( \Delta \), only rather small effects are seen for the \( \pi \) for values of \( m_\pi \) around 600 MeV. The study of the effects due to dynamical quarks, clearly more important at lower pion masses and high \( Q^2 \), is an area where further work is necessary.

This concludes our investigation of the pion form factor at \( T = 0 \). In the next chapter, we will focus on the changes this observable might undergo when the interacting quark and anti-quark are embedded in a heat bath of finite temperature.