Isospin-breaking Effects in Octet and Decuplet Baryon Masses

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We present work designed to compute baryon masses on $N_f = 2 + 1$ CLS ensembles including isospin-breaking effects due to non-degenerate light quark masses and electromagnetic interactions. These effects are determined at leading order via a perturbative expansion around the iso-symmetric theory. We furthermore apply a group-theoretical operator construction for the various interpolators describing the different members of the baryon octet and decuplet based on a classification by spin, parity, and flavor content.

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1. Introduction

We are in an era of precision lattice QCD physics, where contributions from QED and strong-isospin-breaking can no longer be ignored. An example where these contributions are of significant importance is in the lattice determination of the anomalous magnetic moment of the muon $(g-2)_\mu$. Commonly, one of the largest uncertainties in any lattice determination of $(g-2)_\mu$ comes from the scale setting and it is of great importance that a calculation has the physical scale set accurately (below 1%) incorporating QED and isospin-breaking effects

As ensembles for lattice QCD are often generated for the isosymmetric theory QCD_{iso}, perturbative methods were developed to incorporate isospin-breaking effects into calculations on these isosymmetric ensembles [1, 2]. The goal of this project is to reduce the contribution of isospin-breaking effects to the uncertainty of the lattice scale a for $N_f = 2 + 1$ CLS ensembles.

In ref. [3], the lattice scale for the of CLS ensembles was determined using a combination of pion and kaon decay constants. While the final result has a total error at the level of 1%, the incorporation of isospin-breaking corrections turns out to be quite difficult [4]. In this project, we investigate the prospects of precision scale setting using the masses of the lowest-lying baryon octet and decuplet, for which isospin-breaking effects are simpler to incorporate.

2. Inclusion of Perturbative Isospin-breaking Effects by Reweighting

The procedure for the calculation of isospin-breaking corrections to the hadron masses follows the perturbative approach introduced by the RM123 collaboration [1, 2]. Here, the QCD+QED action S described by the set of parameters $\varepsilon = (\beta, e^2, m_u, m_d, m_s)$ (the inverse QCD coupling, the squared QED coupling, and the masses of the up, down, and strange quarks) is expanded around the isospin-symmetric action $S^{(0)}$ with parameters $\varepsilon^{(0)} = (\beta^{(0)}, 0, m_{ud}^{(0)}, m_{ud}^{(0)}, m_s^{(0)})$ in terms of these parameters. $S^{(0)}[U, \psi, \bar\psi] = S_g^{(0)}[U] + S_q^{(0)}[U, \psi, \bar\psi]$ here denotes an isospin-symmetric action consisting of the Lüscher-Weisz action $S_g^{(0)}$ for the gauge fields and an $O(a)$ improved action $S_q^{(0)}$ for Wilson fermions with $N_f = 2 + 1$ flavors [5]. In this work we use gauge ensembles simulated by the CLS collaboration. The QCD+QED action can be divided into three parts, a QCD gauge action, a QED gauge action, and a quark action:

$$S[U, A, \psi, \bar\psi] = S_g[U] + S_\gamma[A] + S_q[U, A, \psi, \bar\psi]$$

For the QED gauge action in finite volume, we use the non-compact QED_L prescription [6] in Coulomb gauge, which introduces an infrared regularisation by eliminating the zero-momentum modes of the photon field by setting

$$\sum_{\mathbf{x}} A^{\mathbf{x},t} \equiv 0$$

on every timeslice t.

In this setup, expectation values for operators in the full theory, i.e.

$$
\begin{aligned}
\langle O \rangle_S &= \frac{1}{Z} \int \mathcal{D}U \mathcal{D}A \mathcal{D}\psi \mathcal{D}\bar{\psi} \, O[U, A, \psi, \bar{\psi}] e^{-S[U, A, \psi, \bar{\psi}]} \\
&= \frac{1}{Z} \int \mathcal{D}U \underbrace{\left(\frac{1}{Z_{q\gamma}[U]} \int \mathcal{D}A \mathcal{D}\psi \mathcal{D}\bar{\psi} \, O[U, A, \psi, \bar{\psi}] e^{-S_\gamma[A] - S_q[U, A, \psi, \bar{\psi}]} \right)}_{=: \langle O \rangle_{S_{q\gamma}}[U]} \underbrace{Z_{q\gamma}[U] e^{-S_g[U]}}_{=: \exp(-S_{\text{eff}}[U])}
\end{aligned}
\tag{1}
$$

can be expressed in terms of those in isosymmetric QCD by reweighting [7, 8]:

$$
\langle O \rangle_S = \frac{\frac{1}{Z_{\text{eff}}^{(0)}} \int \mathcal{D}U \, \langle O \rangle_{S_{q\gamma}}[U] \frac{\exp(-S_{\text{eff}}[U])}{\exp\left(-S_{\text{eff}}^{(0)}[U]\right)} e^{-S_{\text{eff}}^{(0)}[U]}}{\frac{1}{Z_{\text{eff}}^{(0)}} \int \mathcal{D}U \, \frac{\exp(-S_{\text{eff}}[U])}{\exp\left(-S_{\text{eff}}^{(0)}[U]\right)} e^{-S_{\text{eff}}^{(0)}[U]}} = \frac{\left\langle R \, \langle O \rangle_{S_{q\gamma}} \right\rangle_{S_{\text{eff}}^{(0)}}}{\langle R \rangle_{S_{\text{eff}}^{(0)}}} \quad ,
\tag{2}
$$

where R denotes the reweighting factor

$$
R = \frac{\exp(-S_{\text{eff}})}{\exp\left(-S_{\text{eff}}^{(0)}\right)} = \frac{\exp(-S_g) Z_{q\gamma}}{\exp\left(-S_g^{(0)}\right) Z_q^{(0)}},
\tag{3}
$$

which replaces the Boltzmann weight associated with the effective action of QCD_{iso} by its counterpart in QCD+QED. The effective actions are defined as

$$
S_{\text{eff}}[U] = S_g[U] - Z_{q\gamma}[U] = S_g[U] - \log\left(\int \mathcal{D}A \mathcal{D}\psi \mathcal{D}\bar{\psi} \, e^{-S_\gamma[A] - S_q[U, A, \psi, \bar{\psi}]} \right)
$$

$$
S_{\text{eff}}^{(0)} = S_g^{(0)}[U] - Z_q^{(0)}[U] = S_g^{(0)}[U] - \log\left(\int \mathcal{D}\psi \mathcal{D}\bar{\psi} \, e^{-S_q^{(0)}[U, \psi, \bar{\psi}]} \right).
$$

To evaluate the expectation value $\langle O \rangle_{q\gamma}$ and the reweighting factor R in eq. (2) we use perturbation theory and expand the latter expressions in terms of the parameters

$$
\begin{aligned}
\Delta\varepsilon &= \varepsilon - \varepsilon^{(0)} = (\Delta\beta, e^2, \Delta m_u, \Delta m_d, \Delta m_s) \\
&= (\beta - \beta^{(0)}, e^2, m_u - m_{ud}^{(0)}, m_d - m_{ud}^{(0)}, m_s - m_s^{(0)})
\end{aligned}
$$

around $\varepsilon^{(0)}$. Operators that depend on the QED gauge links $\exp(iaeQA)$, where Q denotes the matrix of quark charges, also have to be expanded in e, i.e. $O = O^{(0)} + eO^{(\frac{1}{2})} + \frac{1}{2}e^2 O^{(1)} + O(e^3)$.

3. Baryon Operators

The operator bases used for the various baryons considered in this work were first introduced in Ref. [9]. These operators are obtained from a group-theoretical construction of the coefficients λ for a baryonic interpolator

$$
O_B = \sum_{a,b,c,f_i,\mu_j} \varepsilon_{abc} \lambda_{f_1, f_2, f_3}^{\mu_1, \mu_2, \mu_3} q_{\mu_1}^{f_1, a} q_{\mu_2}^{f_2, b} q_{\mu_3}^{f_3, c},
$$

where $f_i \in u, d, s$ label the flavor of the quarks, a, b, c are color indices, and μ_i are Dirac-spinor indices. In this project we use Wuppertal-smeared fields, i.e. $q = W\Psi$, where Ψ is a point source and W is an APE-smeared smearing operator.

This construction distinguishes different baryons by their symmetries w.r.t the quark flavors f_i and the flavors themselves. For each flavor symmetry, a set of operators based on the third spin component and parity are constructed from a tensor product of Weyl spinors. The only differences between the operators we use and those in [9] are their normalization and that we do not make use of the totally symmetric Σ and Ξ operators. Furthermore, we do not use the H-irreps of the nucleon and (in the isosymmetric case) Λ, as well as the G_1-irreps of the Δ and Ω states since we are only interested in the ground state energies.

These operators are constructed in the Dirac-Pauli basis, in which the parity operator only acts on the first two indices of a Dirac spinor and the spin-z operator only acts on the last two spinor indices, which allows for a convenient construction of the operators based on parity and spin-z eigenvalues in terms of Weyl spinors χ, ξ such that the Dirac spinor is given by $\psi = \chi \otimes \xi$:

$$\mathcal{P}\psi(\mathbf{x}, t) = \gamma_0 \psi(-\mathbf{x}, t) = ((\sigma_3 \chi) \otimes \xi)(-\mathbf{x}, t),$$
$$S_z \psi(\mathbf{x}, t) = -i\gamma_1 \gamma_2 \psi(\mathbf{x}, t) = \chi \otimes (\sigma_3 \xi)(\mathbf{x}, t).$$

Using this fact, baryonic operators are constructed from three Weyl spinors on which the parity operator acts and three Weyl spinors defining the spin of the baryon. The tensor product of different symmetrizations of these combinations of three Weyl spinors then define the baryon operators. Since the baryon operators are already antisymmetric w.r.t their color indices, the combined symmetry of spinor and flavor indices has to be chosen such that the operators are antisymmetric under the exchange of two quarks. As the different baryons are classified according to their flavor symmetries, the Dirac indices thus have to make the operators symmetric or mixed-symmetric under simultaneous exchange of flavor and spin indices.

In total, this procedure results in 116 different operators: 58 for each parity eigenvalue. Because more than one of these operators are expected to have overlap with the same ground state, this allows us to perform a GEVP in order to better control the excited states [10, 11]. The sizes of the correlator matrices for the different baryons are listed in table 1, with each baryon having one correlator matrix for each spin-z eigenvalue.

Table 1: Sizes of the correlator matrices for each particle.

	N	Λ	Σ/Ξ	Δ/Ω	Σ^*/Ξ^*	Σ-Λ-mixing	Σ^*-Λ-mixing
Correlator size	3×3	4×4	3×3	2×2	2×2	7×7	2×2

4. Baryonic two-point functions

As we are aiming for the determination of baryon masses, we consider baryonic two-point functions consisting of zero-momentum projected baryonic creation and annihilations operators $\overline{\mathcal{B}} = \overline{B\Psi\Psi\Psi}$ and $\mathcal{B} = B\Psi\Psi\Psi$. In the following, we assume that $\overline{\mathcal{B}}$ and $\mathcal{B}$ do not depend on e, i.e. $\overline{\mathcal{B}} = \overline{\mathcal{B}}^{(0)}$ and $\mathcal{B} = \mathcal{B}^{(0)}$. In particular, we may apply QCD-covariant but not QCD+QED-covariant

operator smearing. The latter would lead to contributions from $\overline{\mathcal{B}}^{(\frac{1}{2})}$, $\overline{\mathcal{B}}^{(1)}$, $\mathcal{B}^{(\frac{1}{2})}$ and $\mathcal{B}^{(1)}$ and hence to additional diagrams.

As an example, the expansion of baryonic correlation functions is shown in fig. 1, in which sequential propagators are used in the first-order terms. The full expansion also contains diagrams
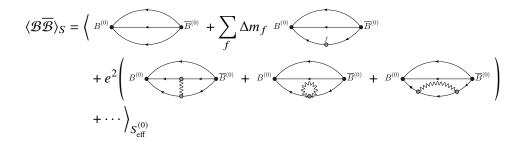

Figure 1: Diagrammatic expansion of QCD+QED correlation functions in terms of isospin-breaking parameters around correlators in QCD$_{\text{iso}}$. The index f counts the different quark flavors.

with quark-disconnected parts and corrections acting in the sea quark sector. However, in this project we neglect isospin-breaking effects in the sea quarks (for the time being) and we set $\Delta\beta$ to 0. As a consequence, only quark-connected contributions remain and $R = 1$ in eq. (2). Nonetheless, we calculate the diagrams with a photon line connected to one of the valence quarks in case we decide to include the disconnected contributions at a later stage since they are needed for diagrams in which a sea quark electromagnetically interacts with a valence quark. Note that in section 5 only contributions shown in fig. 1 are discussed. However, the additional diagrams can trivially be incorporated into the optimizations described, which moreover remove any significant overhead arising from the additional computation of these diagrams.

In order to extract the mass of the lowest state incorporated in a baryonic two-point function, we consider the asymptotic time dependence $C(t_2, t_1) = ce^{-m(t_2-t_1)}$. Expanding the latter in terms of the isospin-breaking parameters $X = X^{(0)} + \sum_i \Delta\varepsilon_i X_i + O(\Delta\varepsilon^2)$ with $X \in \{c, m, C\}$, one finds the zeroth- and first-order contributions

$$C^{(0)}(t_2, t_1) = c^{(0)} e^{-m^{(0)}(t_2-t_1)},$$
$$C_i^{(1)}(t_2, t_1) = \left(c_i^{(1)} - c^{(0)} m_i^{(1)}(t_2 - t_1)\right) e^{-m^{(0)}(t_2-t_1)}.$$

$m^{(0)}$ can then be reconstructed from the usual definition of the effective mass

$$(am_{\text{eff}})^{(0)}(t_2, t_1) := \log\frac{C^{(0)}(t_2, t_1)}{C^{(0)}(t_2 + a, t_1)},$$

with the analogous definition for the first-order terms

$$(am_{\text{eff}})_i^{(1)}(t_2, t_1) := \frac{C_i^{(1)}(t_2, t_1)}{C^{(0)}(t_2, t_1)} - \frac{C_i^{(1)}(t_2 + a, t_1)}{C^{(0)}(t_2 + a, t_1)}.$$

5. Computational Optimizations

We compute correlation functions using the operators described in section 3 with a program written in C++ making use of the libraries OpenQCD for quark propagator inversions and QDP++ for the remaining computations. For better statistics for the same amount of computing time, we apply all-mode averaging [12].

As the chosen set of operators described in section 3 yields a large number (528) of non-vanishing correlator matrix entries, the contractions can easily become a bottleneck in the computation of the different correlators, especially in the case of isospin-breaking corrections. Therefore, a number of optimizations have been applied to the production code in order to keep the computational costs small compared to the inversions.

First, the contractions are simplified algebraically by identifying the up and down quark propagators with the light quark l used in the simulations, which is possible as we use isospin-symmetric ensembles. A similar simplification is done for up and down propagators including a photon vertex: In the contractions, these terms come with a factor $e_f e$ for each three-point-vertex or $(e_f e)^2$ in the case of a four-point-vertex, where e is the electromagnetic coupling and

$$
e_f = \begin{cases} \frac{2}{3} & f = u \\ -\frac{1}{3} & f \in \{d, s\} \end{cases} .
$$

Thus, in a diagram with photon interactions, the product of the fractional charges of the quarks at each photon vertex yields simply a prefactor for the contractions with S_d and S_u replaced by S_l. Note, that the charge multiplicity e_f is already absorbed into the definition of the vertices in fig. 1.

This leaves 101580 individual, color-contracted terms of the form:

$$
T_{\mu_1 \mu_2 \mu_3}^{f_1 f_2 f_3} = \sum_{\substack{a,b,c \\ a',b',c'}} \varepsilon_{abc} \varepsilon_{a'b'c'} \lambda_{f_1 f_2 f_3}^{\mu_1 \mu_2 \mu_3} \lambda_{f_1 f_2 f_3}^{\mu_4 \mu_5 \mu_6} S_{\mu_1 \mu_4}^{f_1, aa'} S_{\mu_2 \mu_5}^{f_2, bb'} S_{\mu_3 \mu_6}^{f_3, cc'} , \tag{4}
$$

which divide into 8304 isosymmetric contributions, 38316 contributions from mass detuning, and 54960 from QED corrections.

However, many of these terms appear in multiple contractions (possibly differing in the coefficients λ), enabling a reduction of the computational cost by reusing these terms after their first computation. This reduces the number of terms to be computed to 10104 unique terms of the form

$$
\tilde{T}_{\mu_1 \mu_2 \mu_3}^{f_1 f_2 f_3} = \sum_{\substack{a,b,c \\ a',b',c'}} \varepsilon_{abc} \varepsilon_{a'b'c'} S_{\mu_1 \mu_4}^{f_1, aa'} S_{\mu_2 \mu_5}^{f_2, bb'} S_{\mu_3 \mu_6}^{f_3, cc'}
$$

such that all correlators can be expressed as linear combinations of these unique terms. This, however, leads to the next challenge: since each term resembles a complex field on the lattice, this is still an unreasonable amount of data to hold in memory at once, especially on large ensembles. This problem can be circumvented by making use of the fact that each correlator has a fixed combination of flavor indices (f_1, f_2, f_3), where we count the sequential propagators from isospin-breaking contributions as separate flavors so that there are a total of 25 different flavor combinations. One can therefore split the set of correlators into much smaller subsets that can be computed in one go

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without the need of keeping the terms in memory for any other subset. These small subsets then contain at most 640 unique terms, which is much more manageable.

Further optimizations were necessary due to the nature of the QDP++ library used for the computation of the contractions. This library is optimized for matrix-based computations on the lattice, but has rather slow routines for retrieving data based on color or spin indices. To avoid these routines, propagators are saved as `std::vector<std::vector<LatticeColorMatrix>>`, so that QDP++'s `peekSpin`-routine only needs to be called 16 times per propagator in order to store the propagator in this format.

Once all propagators for a given flavor combination are calculated, a lookup table for all color-contracted terms is constructed for that flavor combination. This lookup table is finally used to calculate the contractions. It was found to be beneficial, performance wise, to use precompiled functions that return the complete contraction as a single expression in terms of the elements of the lookup table. An example for such a function calculating the contraction for a simple isospin-symmetric nucleon correlator would take references to a `std::map<std::tuple<int, int, int, int, int, int>, LatticeComplex> map` and a `LatticeComplex result` and perform the following computation:

```
result =  3.0 * map.at(std::make_tuple(0, 0, 0, 0, 1, 1))
        - 3.0 * map.at(std::make_tuple(0, 0, 0, 1, 1, 0));
```

The factors `3.0` and `-3.0` correspond to the product of the λ-coefficients in eq. (4), `map` is the above mentioned lookup table which uses keys in the form of a tuple containing the six spinor indices identifying the unique term needed for the contraction. The flavor indices are not mentioned here, since the correlators are already split up according to the flavor index combination, for each of which a set of such functions is defined.

6. Conclusion and Outlook

We have presented our calculational framework for the inclusion of isospin-breaking effects for baryon correlators using isosymmetric CLS ensembles, for which we employ a perturbative method [1, 2]. For the baryon operators, we use a construction based on parity and symmetries in flavor and spinor indices [9] which gives rise to several correlator matrices for the different baryons. We have implemented several optimizations to deal with the vast amount of correlators to be computed.

We have tested our code on an ensemble (A654) of size 48×24^3 with antiperiodic temporal boundary conditions. Preliminary results for the single nucleon correlator suggest that we expect a statistical uncertainty below 1%.

Over the course of the next months, we intend to perform a spectroscopic analysis of the different correlators we have for A654 including the use of the GEVP method. Moreover, we are going to generate correlator data for larger 128×64^3 ensembles, namely D450 and D452, to perform similar analyses on these ensembles.

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