Excited states in lattice QCD with the stochastic LapH method

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Abstract. Progress in computing the spectrum of excited baryons and mesons in lattice QCD is described. Results in the zero-momentum bosonic \( I = \frac{1}{2} \), \( S = 1 \), \( T_{1u} \) symmetry sector of QCD using a correlation matrix of 58 operators are presented. All needed Wick contractions are efficiently evaluated using a stochastic method of treating the low-lying modes of quark propagation that exploits Laplacian Heaviside quark-field smearing. Level identification using probe operators is discussed.

1. Introduction

In a series of papers \cite{1–7}, we have been striving to compute the finite-volume stationary-state energies of QCD using Markov-chain Monte Carlo integration of the QCD path integrals formulated on a space-time lattice. In this talk, our progress towards this goal is described. First results in the zero-momentum bosonic \( I = 1 \), \( S = 0 \), \( T_{1u}^+ \) symmetry sector of QCD using a correlation matrix of 56 operators were recently presented in Ref. \cite{7}. Here, preliminary results in the zero-momentum bosonic \( I = \frac{1}{2} \), \( S = 1 \), \( T_{1u} \) sector using a correlation matrix of 58 operators are presented. Nine spatially-extended single-kaon operators are used, and 49 two-meson operators involving a wide variety of light isovector, isoscalar, and strange meson operators of varying relative momenta are included. All needed Wick contractions are efficiently evaluated using a stochastic method of treating the low-lying modes of quark propagation that exploits Laplacian Heaviside quark-field smearing. Given the large number of levels extracted, level identification becomes a key issue.

2. Energies from correlations of single-meson and two-meson operators

The stationary-state energies in a particular symmetry sector can be extracted from an \( N \times N \) Hermitian correlation matrix \( C_{ij}(t) = \langle 0 | \mathcal{O}_i(t + t_0) \mathcal{O}_j(t_0) | 0 \rangle \), where the \( N \) operators \( \mathcal{O}_j \) act on the vacuum to

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create the states of interest at source time $t_0$ and are accompanied by conjugate operators $O_j$ that can annihilate these states at a later time $t + t_0$. Estimates of $C_{ij}(t)$ are obtained with the Monte Carlo method using the stochastic LapH method [5] which allows all needed quark-line diagrams to be computed. The operators that we use have been described in detail in Refs. [1, 5, 6]. All of our single-hadron operators are assemblages of basic building blocks which are gauge-covariantly-displaced, LapH-smeared quark fields. We simplify our spectrum calculations as much as possible by working with single-hadron operators that transform irreducibly under all symmetries of a three-dimensional cubic lattice of infinite extent or finite extent with periodic boundary conditions. We construct our two-hadron operators as superpositions of single-hadron operators of definite momenta. The details are described in Ref. [6]. This approach is efficient for creating large numbers of two-hadron operators, and generalizes to three or more hadrons. We utilize multi-hadron operators with a variety of different relative momenta.

In finite volume, all energies are discrete so that each correlator matrix element has a spectral representation of the form $C_{ij}(t) = \sum_n Z_i^{(n)} Z_j^{(n)*} e^{-E_n t}$, with $Z_j^{(n)} = \langle 0 | O_j | n \rangle$, assuming temporal wrap-around (thermal) effects are negligible. It is not practical to extract the $E_n$ and $Z_j^{(n)}$ from fits to all of our correlator matrix elements. Instead, we rotate the matrix so that its off-diagonal elements are statistically consistent with zero for large time separations. The rotated correlator is given by $G(t) = U^† C(t) U C(t) U^† C(t) U$, where the columns of $U$ are the orthonormalized eigenvectors of $C(t) U C(t) U^†$ for a judicious choice of $t_0$ and $\tau_D$. Rotated effective masses can then be defined by

$$m_G^{(n)}(t) = \frac{1}{\Delta t} \ln \left( \frac{G_{nn}(t)}{G_{nn}(t + \Delta t)} \right),$$

using $\Delta t = 3$. These tend to the lowest-lying $N$ stationary-state energies produced by the $N$ operators. Correlated-$\chi^2$ fits to the estimates of $G_{nn}(t)$ using the forms $A_n e^{-E_n t}(1 + B_n e^{-\Delta \xi t})$ yield the energies $E_n$ and the overlaps $A_n$ to the rotated operators for each $n$.

We are currently focusing on three Monte Carlo ensembles: (A) a set of 412 gauge-field configurations on a large $32^3 \times 256$ anisotropic lattice with a pion mass $m_\pi \sim 240$ MeV, (B) an ensemble of 551 configurations on an $24^3 \times 128$ anisotropic lattice with a pion mass $m_\pi \sim 390$ MeV, and (C) an ensemble of 584 configurations on an $24^3 \times 128$ anisotropic lattice with a pion mass $m_\pi \sim 240$ MeV. We refer to these ensembles as the $(32^3|240)$, $(24^3|390)$, and $(24^3|240)$ ensembles, respectively.

Here, we focus on the resonance-rich $I = \frac{1}{2}$, $S = 1$, $T_{1u}$ channel of total zero momentum. This channel has odd parity, and contains the spin-1 and spin-3 mesons. A partial sampling of our “first-pass” results for the $(24^3|390)$ ensemble obtained from a $58 \times 58$ correlation matrix is presented in Fig. 1. The results shown here are not finalized yet. We are still varying the fitting ranges to improve the $\chi^2$, as needed in some instances. We are investigating the effects of adding more operators, and we are even still verifying our analysis/fitting software. However, these figures do demonstrate that the extraction of a large number of energy levels is indeed possible, and the plots indicate the level of precision that can be attained with our stochastic LapH method. Keep in mind that we have not included any three-meson operators in our correlation matrix.

With such a large number of energies extracted, level identification becomes a key issue. Level identification must be inferred from the $Z$ overlaps of our probe operators. We first focus our efforts on identifying the levels that dominate the finite-volume stationary states expected to evolve into the single-meson resonances in infinite volume. We view such states as “resonance precursor states”. To accomplish this, we utilize “optimized” single-hadron operators as our probes. We first restrict our attention to the $9 \times 9$ correlator matrix involving only the 9 chosen single-hadron operators. We then perform an optimization rotation to produce so-called “optimized” single-hadron (SH) operators $\tilde{O}_j$, which are linear combinations of the 9 original operators. We order these SH-optimized operators
Figure 1. Rotated effective masses $m_{(n)}(t)$ (see Eq. (1)) for the 12 lowest-lying energy levels in the zero-momentum bosonic $I = \frac{1}{2}, S = 1, T_{1u}$ channel for the $(24^3 \times 390)$ ensemble using 9 single-meson operators, 25 kaon+isovector operators, 12 kaon+$(\pi u + d d)$-isoscalar operators, and 12 kaon+$s s$-isoscalar operators. The two horizontal dashed lines in each plot indicate the best-fit energy from the correlated-$\chi^2$ fits. The red dashed-dotted line in each plot shows the best-fit two-exponential function. Fit results and qualities are also listed in each plot. Higher-lying levels cannot be shown here due to page limitations. Over 50 energies were extracted.

Figure 2. Overlaps $|\widetilde{Z}_j(n)|^2$ of our “optimized” single-hadron operator $\widetilde{O}_j$ against the eigenstates labelled by $n$. The overall normalization is arbitrary in each plot.

according to their effective mass plateau values, then evaluate the overlaps $|\widetilde{Z}_j(n)|^2$ for these SH-optimized operators using our analysis of the full $58 \times 58$ correlator matrix. The results are shown in Fig. 2.

The first plot shows that the lowest-lying SH-optimized operator produces level 0 and very little else. Hence, we identify level 0 with the lowest-lying resonance precursor state, expected to be the $K^*(892)$. The second plot shows that this operator produces mainly level 12. Hence, we identify level 12 as the dominant state that is the precursor of the first-excited resonance in this channel. We summarize
Figure 3. Left: masses, as ratios with respect to 3/5 of the Ω baryon mass \( m_\Omega \), of the dominant finite-volume isovector \( T_{1u} \) stationary states expected to evolve into the single-meson resonances in infinite volume, computed using our 58 × 58 correlation matrix for the (24^3|390) ensemble. The vertical thickness of each box indicates its statistical uncertainty. The hollow boxes at the top show higher-lying states that we extract with less certainty due to the expected presence of lower-lying two-meson states that have not been taken into account. Right: the analogous plot for the isovector zero-strangeness \( T_{1u}^+ \) channel, the superscript indicating \( G \)-parity.

our single-hadron spectrum (the eigenstates dominated by the resonance precursor states) in Fig. 3. This figure shows the masses as a ratio of 3/5 of the Ω baryon mass. Given that our pion mass is around 390 MeV and that our states are extracted in finite volume, precise agreement with experiment is certainly not expected. These results are compared to the analogous results in the isovector nonstrange \( T_{1u}^+ \) channel from Ref. [7]. Again, these results are preliminary, and we mention that three and four meson states are not taken into account at all.

3. Conclusion

In this talk, our progress in computing the finite-volume stationary-state energies of QCD was described. Preliminary results in the zero-momentum bosonic \( I = \frac{1}{2}, S = 1, T_{1u} \) symmetry sector of QCD using a correlation matrix of 58 operators were presented. All needed Wick contractions were efficiently evaluated using the stochastic LapH method. Issues related to level identification were discussed. This work was supported by the U.S. NSF under awards PHY-0510020, PHY-0653315, PHY-0704171, PHY-0969863, and PHY-0970137, and through TeraGrid/XSEDE resources provided by TACC and NICS under grant numbers TG-PHY100027 and TG-MCA075017.

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