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QCD inequalities for hadron interactions

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We derive generalizations of the Weingarten-Witten QCD mass inequalities for particular multihadron systems. For systems of any number of identical pseudoscalar mesons of maximal isospin, these inequalities prove that near threshold interactions between the constituent mesons must be repulsive and that no bound states can form in these channels. Similar constraints in less symmetric systems are also extracted. These results are compatible with experimental results (where known) and recent lattice QCD calculations, and also lead to a more stringent bound on the nucleon mass than previously derived, $m_N \geq \frac{5}{2} m_x$.

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Analytic relationships between low-energy hadronic quantities are difficult to obtain in quantum chromodynamics (QCD) because it is a strongly interacting field theory, and only a few such relationships are known. Consequently, the various inequalities between hadron masses that have been derived by Weingarten [1], Witten [2], and (under some assumptions) by Nussinov [3] have an important place in our understanding of QCD. The rigorous relations can be summarized by stating that the pion is the lightest colorless state of nonzero isospin [1] ($m_N \geq m_x$ for $X$ being any $I \geq 1$ isospin-charged meson), that the pion electromagnetic mass difference $m_{\pi^+} - m_{\pi^0}$ is positive [2] and that baryons are heavier than pions, $m_B \geq m_x$ [1,4]. The status of QCD inequalities is reviewed in Ref. [5]. The known results concern a relatively small number of static quantities, and it is important to consider whether further relations exist. In this direction, Nussinov and Sathiapalan [6] found that in QCD motivated models there are relationships between scattering lengths in various two-particle channels, and Gupta et al. [7,8] showed that an unphysical combination of $\pi\pi$ interactions is attractive. Finally, Alfaro et al. [9] showed that relationships existed between $K \to \pi$ matrix elements of various four-quark operators. In this Letter, we demonstrate that there are additional rigorous QCD inequalities that pertain to the spectrum of particular physical, multihadron systems and thereby to the nature of the corresponding hadronic interactions. As simple examples, we prove that there are no bound states in the $I = 2\pi^+\pi^-$ or $I = 3/2\pi^-K^+$ channels and also improve on a previous baryon-meson mass inequality, showing that $m_N \geq \frac{7}{5} m_x$. As with the original inequalities, an experimental demonstration that these inequalities are violated would strongly suggest that QCD does not describe the strong interaction (modulo possible effects of electroweak interactions).

A central observation of Vafa and Witten [4] is that the measure of the QCD functional integrals that define QCD correlation functions is positive definite in the absence of a $\theta$ term or baryon chemical potential (we will ignore these cases throughout this work). After integrating over the quark degrees of freedom, the functional integration measure can be expressed as

$$d\mu = \prod_{x,\mu,\alpha} dA_{\mu}^\alpha(x) e^{-S_{YM}[A]} \prod_{f} \det [\mathcal{D} + \tilde{m}_f],$$

where $A_\mu$ represents the gauge field, $\mathcal{D} = \mathcal{D}[A]$ is the bare quark mass of flavor $f$, and $S_{YM} = \frac{1}{2} \int d^4x \text{Tr}(F_{\mu
u}F_{\mu
u})$ is the Yang-Mills action with $F_{\mu
u} = [D^\mu, D^\nu]$. Throughout our discussion, we use a Euclidean metric; for the correlators that we consider, analytic continuation to Minkowski space is straightforward. Correlation functions involving field operators at $n$ spacetime points are defined as

$$\langle \hat{O}(x_1, \ldots, x_n) \rangle = \frac{1}{Z} \int d\mu \hat{O}(x_1, \ldots, x_n),$$

where $Z = \int d\mu$, and the operator $\hat{O}$ results from the operator $\hat{O}$ after integration over quark fields. These functional integrals are only defined after the imposition of a regulator, and we assume the use of a regulator that does not spoil positivity [1,4]. As a consequence of the positivity of the measure, field independent relations that are shown to hold for any particular gauge field configuration also hold for the integrated quantity, the corresponding correlation function. Vafa and Witten used measure positivity to derive the celebrated result that vector symmetries do not break spontaneously.

In related work, Weingarten [1] considered correlation functions from which meson and baryon masses can be determined, and made use of measure positivity and the Cauchy-Schwarz and Hölder inequalities to show that relationships exist between the corresponding functional integrals. The inequalities show that $m_x \leq m_X$, and $m_N \geq (N_f - 2)/(N_f - 3) m_x$ for a theory with $N_f \geq 6$ flavors. Using a further constraint on the spectrum of the inverse of the Dirac operator, shown to hold in Ref. [4], this latter...
constraint was extended to $m_N \geq m_\pi$, independent of the number of flavors.

Our analysis shares similarities with the approaches discussed above, but it also makes use of a novel eigenvalue decomposition of correlation functions. We begin by considering an $I = I_z = n$ many-$\pi^+$ correlator of the form

$$
\left\langle \Omega \left| \prod_{i=1}^{n} \gamma_5 \bar{u}(x_i) \prod_{j=1}^{n} dy_5 \bar{u}(y_j) \right| \Omega \rightangle,
$$

where $|\Omega\rangle$ is the vacuum state and the clusters of points $\{x_i\}$ (sources) and $\{y_j\}$ (sinks) are taken to be well separated in Euclidean space. The combination $dy_5 \bar{u}(y)$ is an interpolating operator that creates the quantum numbers of a $\pi^+$ meson. We specify to vanishing total momentum by separately summing over the spatial components of the $y_j$ coordinates and for simplicity set the temporal components $x_i^0 = 0 \quad \forall \ i$ and $y_j^0 = t \quad \forall \ j$ and allow for some of the source locations to be the same (nonzero correlators result provided that $4N_c$ or less quark fields are placed at the same spacetime point). This leads to

$$
C_n \equiv C_n(x_1, \ldots, x_n; t; \mathbf{P} = 0) = \left\langle \Omega \left| \prod_{i=1}^{n} \gamma_5 \bar{u}(x_i, 0) \left[ \sum_{y} dy_5 \bar{u}(y, t) \right] \right| \Omega \rightangle.
$$

As shown in Refs. [10,11], these correlation functions can be written in terms of products of traces of powers of the matrix

$$
\Pi_A = \begin{pmatrix}
P_{1,1} & P_{1,2} & \cdots & P_{1,N_a} \\
P_{2,1} & \ddots & & \vdots \\
\vdots & \ddots & \ddots & \vdots \\
P_{N_a,1} & \cdots & \cdots & P_{N_a,N_a}
\end{pmatrix},
$$

where $N_a$ is the number of source locations being considered, the $4N_c \times 4N_c$ blocks are given by

$$
P_{i,j}(t) = \sum_y S_u(x_i, 0; y, t) \gamma_5 S_d(y, t; x_j, 0) \gamma_5,
$$

and $S_u$ and $S_d$ are propagators for the up and down quarks, respectively. The subscript $A$ indicates that the matrix depends on the background gauge field and $\Pi_A$ is a matrix of dimension $N = 4N_c N_a$ and by increasing $N_a$, this can be taken to infinity.

This can be further simplified in the isospin limit where the up and down quark propagators are the same, $S_u = S_d$, and by using the $\gamma_5$ the roots of the Hermiticity of the Dirac operator that implies that $\gamma_5 S_d(y, x) \gamma_5 = S_d'(x, y)$ so that the $P_{i,j}$ take the form

$$
P_{i,j}(t) = \sum_y S_u(x_i, 0; y, t) S_d'(x_j, 0; y, t).
$$

Consequently, we see that $\Pi_A$ is a non-negative definite Hermitian matrix, as are all its diagonal subblocks. In Ref. [10], it was shown that the contributions to the correlation functions $C_j$ for $j \leq N$ determined on a given gauge configuration arise as coefficients of the characteristic polynomial

$$
\mathcal{P}_A(\alpha) = \det(1 + \alpha \Pi_A) = \sum_{j=0}^{N} c_j[A] \alpha^j
$$

of the matrix $\Pi_A$. (There are normalization differences between the $c_j$ and $C_j$, and for multiple source locations, the $c_j$ are linear combinations of the $C_j$ with different numbers of interpolators at each source. The spectrum is common to each term in this linear combination.) Since the roots of the characteristic polynomial are determined by the eigenvalues $\pi_i$ of $\Pi_A$, it follows that

$$
c_n[A] = \sum_{i_1 \neq i_2 \neq \ldots \neq i_n = 1} \pi_{i_1} \pi_{i_2} \ldots \pi_{i_n},
$$

Thus $c_1[A] = \sum_{i=1}^{N} \pi_i = \text{tr}[\Pi_A]$, $c_2[A] = \sum_{i=1}^{N} \sum_{j \neq i=1}^{N} \pi_i \pi_j$, $\ldots$, $c_N[A] = \pi_1 \ldots \pi_N = \det[\Pi_A]$. Since these eigenvalues are non-negative, we can bound these expressions by products of the single pion expression by relaxing the restrictions on the summation above. That is,

$$
c_n[A] \leq \sum_{i_1, i_2, \ldots, i_n = 1}^{N} \pi_{i_1} \pi_{i_2} \ldots \pi_{i_n} = \left( \sum_{i=1}^{N} \pi_i \right)^n = c_n^0[A].
$$

From this eigenvalue relation, valid on a fixed background gauge configuration, we can construct the field independent bound, $c_n[A] - c_n^0[A] \leq 0$, that holds for all $A_n'$. Measure positivity then implies that this relation holds at the level of QCD correlators. (We note that the results hold for lattice QCD discretizations that preserve measure positivity such as domain-wall [12] and overlap fermions [13,14], or Wilson fermions [15] with even $N_f$.) The large separation behavior of $\langle c_n \rangle$ is governed by the energy of the lowest energy eigenstates of the system, $\langle c_n \rangle \sim \exp(-E_n^{(0)}/t)$. We also note that $\langle c_n^0 \rangle \leq \sigma \langle c_1 \rangle^n$ for some source-sink separation independent $\sigma$. Together, this implies that $E_n^{(0)} \geq nE_1^{(0)} = nm_\pi$ and consequently that there are no bound states possible in these maximal isospin channels. Further, it is also implies that the two-body interactions in these systems are repulsive or vanishing at threshold. This second result follows from the fact that the relations derived above are valid in a finite volume where the energy eigenvalues of two particle systems below inelastic thresholds are determined by the appropriate infinite volume scattering phase shift [16,17]. Since the scattering phase shift near threshold is proportional to the negative of the non-negative definite energy shift, it must correspond to a repulsive or vanishing interaction.
The two-pion results are in accordance with expectations from chiral perturbation theory ($\chi$PT) [18,19] which predicts at next-to-leading order (NLO) that
\[
m_{\pi}^{2NLO} = -2\chi[1 + \chi(3\log\chi - L_{\pi}^{2NLO})],
\]
where $\chi = [m_\pi/4\pi f_\pi]^2$, $f_\pi$ is the pion decay constant, and $L_{\pi}^{2NLO}$ is a particular combination of low-energy constants (LECs) renormalized at scale $\mu = 4\pi f_\pi$. At tree level, this expression is universally negative, and at NLO it remains negative given the phenomenological constraints on $L_{\pi}^{2NLO}$. However, the bounds derived above are statements directly about QCD and do not rely on a chiral expansion, and in fact provide a fundamental constraint on $L_{\pi}^{2NLO}$ (the use of single particle QCD inequalities to constrain $\chi$PT is discussed in Refs. [20,21].) The $\pi\pi$ scattering phase shifts can be experimentally extracted from studies of kaon decays [22–24] and the lifetime of pionium [25], but the direct constraints of the $I = 2$ channel are relatively weak. A chiral and dispersive analysis of experimental data nevertheless allows for a precise extraction [26], giving $m_{\pi N}^{2NLO} = -0.0444(10)$ and lattice QCD calculations [27–33] are in agreement. The sign implies that these results are concordant with the QCD inequalities derived here.

As a corollary, having shown that the $(\pi^+)^n$ systems do not bind, we can follow the discussion of Ref. [5] and strengthen the nucleon mass bound of Weingarten to $m_N \geq \frac{1}{2} m_\pi$. This improves on the bounds of Refs. [1,6,34] as it applies for arbitrary $N_f$ and $N_c$ and the inequality directly involves the pion mass. Furthermore, less complete modifications of the restricted sums in Eq. (9) show also that $E_n^{(0)} \geq E_{n-1}^{(0)} + E_{n}^{(0)}$ for all $j < n$. This then implies that the $I = 3$, $\pi^+\pi^-\pi^+$ interaction is repulsive at threshold, as are the $I = n$, $(\pi^+)^n$ interactions. In principle, the form of these interactions could be computed in the chiral expansion, and the constraints derived here would bound the LECs that enter. Lattice calculations show that the $\pi^+\pi^-\pi^+$ interaction is indeed repulsive [35,36].

The inequalities above concern identical pseudoscalar mesons formed from quarks of equal mass, but they can be generalized in a number of ways. In particular, these inequalities can be extended to the case of unequal quark masses; thereby analogous results can be derived for multiple pion systems away from the isospin limit. Further, by defining
\[
K_{i,j}(t) = \sum_y S_{i}(x_i, 0; y, t) S_{j}(y, t; x_j, 0),
\]
where $S_{i}(x, y)$ is the strange quark propagator, in addition to $P_{i,j}$, correlators containing both $\pi^+$ and $K^+$ mesons can be studied. The matrix $K_{A}$ can be constructed from the $K_{i,j}$ subblocks analogously to Eq. (5). To see how these generalizations arise, we need to examine the spectrum of the relevant matrices. If we denote the eigenvalues and eigenfunctions of the Dirac operator as $\lambda_i$ and $v_i$ respectively, that is $D v_i = \lambda_i v_i$, we can decompose the quark propagators as
\[
S_f = \sum_i \frac{v_i v_i^*}{\lambda_i + m_f} = \sum_i g_i^{(f)} v_i v_i^*,
\]
where $m_f$ is the renormalized quark mass (in what follows, we assume a mass-independent and multiplicatively renormalizable regularization and renormalization scheme) and the matrix $\Pi_A$ as
\[
\Pi_A = \sum_i \pi_i v_i v_i^* = \sum_{i,j} \frac{v_i v_i^* v_j v_j^*}{\lambda_j + m_d},
\]
with a similar expression for $K_A$ [in the second equality for $\Pi_A$, we have used (Coulomb-gauge spatial) completeness as we are integrating over the spatial position of the sink in defining $P_{i,j}$]. Because of the spectral properties of the Dirac operator ($\lambda_i \in \mathbb{R}$ and $\{\lambda_i, \lambda_j\}$ both eigenvalues), the eigenvalues of quark propagators, $g_i^{(f)}$, fall on circles [center $[1/(2m_f), 0], radius 1/(2m_f)$] in the complex plane. For the matrix $\Pi_A$ in the isospin limit, we immediately see that the eigenvalues are real and non-negative as stated above, occupying the interval $[0,1/m_f]$. Away from the isospin limit, $\Pi_A$ and $K_A$ have eigenvalues, denoted $\pi_i$ and $\kappa_i$, respectively, that occur in complex conjugate pairs with non-negative real parts and imaginary parts that are proportional to the mass splitting $|m_i - m_2|$. The locii of these eigenvalues are shown in Fig. 1 for exemplary masses.

The spectral properties [the overlap Dirac operator [13,14], which is $\gamma_5$ Hermitian and has eigenvalues on the circle $(1 + \cos\theta, \sin\theta) \in \mathbb{C}$ for $0 \leq \theta < 2\pi$, is an explicit regulator for which the argument that follows

FIG. 1 (color online). Eigenvalues of $S_\mu$, $S_\mu S_\mu^*$ and $S_\mu S_\mu^*$ for $m_\mu = 1$ and $m_d = 1.5$.
holds] discussed above are sufficient to show that even in the less symmetric cases mentioned previously, the generalizations of the eigenvalue inequality used in Eq. (10) still hold, at least for certain quark mass ratios in systems containing up to \( n = 8 \) particles (for example \( \pi^+\pi^+\pi^+K^+ \)) where we have explicitly checked. (We expect that these results hold for all \( n \) and all mass ratios but have been unable to prove the necessary relations.) To see this, we reconsider the eigenvalue sums that occur in the expressions for correlators [the correlators for \( J\pi^+ \)s and \( KK^+ \)s can be constructed from the expansion of \( \det(1 + \alpha \Pi_k + \beta K)_k \) as discussed in Ref. [37]] with the quantum numbers of \( (\pi^+)^iJ(K)^{n-j} \), denoted \( c_{j,n-j} \). As the simplest example we consider

\[
c_{1,1} \sim \sum_i \frac{\pi_i \kappa_j}{\frac{1}{2}} = \sum_i \pi_i \kappa_j - \sum_i \pi_i \kappa_j, \tag{15}
\]

and shall show that the last sum is positive. This is most easily approached in the \( N \to \infty \) limit in which the eigenvalue sums become continuous integrals. To make our notation simpler, we replace \( \lambda \to \lambda R \) with \( \lambda_R \in \mathbb{R} \) and subsequently drop the subscript. In this case, defining

\[
f_{a,b}(\lambda) = \frac{\lambda^2 + m_a m_b + i\lambda(m_a - m_b)}{(\lambda^2 + m_a^2)(\lambda^2 + m_b^2)}, \tag{16}
\]

and \( \pi(\lambda) = f_{a,d}(\lambda) \) and \( \kappa(\lambda) = f_{a,s}(\lambda) \), we can replace \( \sum_i \pi_i \kappa_j \) by

\[
\int_{-\infty}^{\infty} D\lambda \pi(\lambda) \kappa(\lambda), \tag{17}
\]

where the measure \( D\lambda \) is weighted by the spectral density of the Dirac operator, \( \rho(\lambda) \). Since the spectral density is non-negative, a non-negative integrand results in a non-negative integral. However, the integrand above is only positive definite for some ranges of the ratios \( m_d/m_s \) and \( m_s/m_u \) (we specify to a mass-independent multiplicative renormalization scheme for the quark masses in which these ratios are scale independent; schemes involving a chiral lattice regularizations such as domain-wall fermions and overlap fermions are examples) as is shown for this case in Fig. 2. If the mass ratios are in the allowed region, then \( c_{1,1} \leq c_{1,0} c_{0,1} \) and through the same logic that we employed for \( I = 2 \) \( \pi \pi \pi \) systems, we see that \( E_{\pi^+K^+} \geq m_{\pi^+} + m_{K^+} \), so \( I = 3/2 \) \( \pi^+K^+ \) scattering cannot result in bound states. This result is in agreement with lattice calculations [37–40]. Outside these parameter ranges, the integral has negative contributions at intermediate \( \lambda \) but is positive at large \( \lambda \); given the expectations of the behavior of the spectral density, \( \rho(\lambda) \sim V\lambda^3 \) for large \( \lambda \), this suggests that the integral is always positive in Eq. (17), but this cannot be proven rigorously. For the important cases of \( \pi^+\pi^+ \) at \( m_d \neq m_u \) and \( \pi^+K^+ \), the physical mass ratios [41] are such that the proof is complete, but for example for \( I = 1 \) \( K^+K^+ \) or \( D^+D^+ \), the mass ratios are such that the proof fails.

In a more complicated case, such as \( c_{3,1} \), the subtractions are more involved,

\[
c_{3,1} \sim \sum_{i,j} \sum_{k \neq i,j} \sum_{l 
eq i,j,k} \pi_i \pi_j \pi_k \pi_l
\]

\[= \sum_{i,j,k,l} \sum_{j \neq i} \pi_i \pi_j \pi_k \pi_l - 3 \sum_{i,j,k,l} \pi_i^2 \pi_j \pi_k \pi_l + \pi_i \pi_j \pi_k \pi_l - \sum_{i,j} \pi_i^3 \pi_j \pi_k \pi_l
\]

\[= \sum_{i,j,k,l} \pi_i \pi_j \pi_k \pi_l - \left\{ \sum_{i,j,k} \pi_i^2 \pi_j \pi_k \pi_l + \pi_i \pi_j \pi_k \pi_l \right\}
\]

\[\sim \sum_{i,j,k} (2\pi_i^3 \pi_j^j + 6\pi_i^2 \pi_j \pi_k^j + 3\pi_i^2 \pi_j \pi_k) \tag{18}
\]

However, by again taking the continuous limit and writing the eigenvalue sums as (multiple) integrals, the term in the braces can be proven to be positive for certain values of \( m_d/m_u \) and \( m_s/m_u \), thereby showing \( E_{\pi^+\pi^+\pi^+K^+} \geq 3m_{\pi^+} + m_{K^+} \). The region of guaranteed positivity varies with the number of pions and kaons in the system, but a region exists for all \( c_{i,j,k,l} \).

As a further generalization, we may consider modified correlators where we replace some of the \( \gamma_5 \) matrices in Eq. (4) by other Dirac structures. We can then use the Cauchy-Schwartz inequality to derive the related results.
that the energies of arbitrary $J^P$ states with $I = I_z = n$ are bounded from below by $nm_x$ in the same manner in which Weingarten [1] showed that $m_x \geq m_z$. This does not prohibit bound state formation if the quantum numbers prohibit an $n\pi^+$ state in the given channel (for example $\rho^+\pi^+\rho^+$ with $J^P = 3^-$), but limits the amount of binding that is possible.

In summary, we have shown that the hadron mass inequalities previously derived in QCD have an infinite set of analogues for certain multihadron systems that constrain the nature of the interactions between the constituent hadrons. These results provide important constraints on phenomenological and lattice QCD studies of hadron interactions and serve as fundamental tests of QCD. The scope of the techniques used to derive the original hadron mass inequalities and the new techniques introduced here is more general than the two-point correlation functions considered so far, and there are a number of extensions that may be pursued productively.

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