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We derive the relations necessary for the extraction of matrix elements of multi-hadron systems from finite-volume lattice QCD calculations. We focus on systems of $n \geq 2$ weakly interacting identical particles without spin. These results will be useful in extracting physical quantities from lattice QCD measurements of such matrix elements in many-pion and many-kaon systems.

I. INTRODUCTION

An important goal in nuclear physics is to understand how the presence of a hadronic/nuclear medium modifies the properties of hadrons. Experimentally, there are a number of examples where such modifications are observed and are significant in their effects. The EMC effect [1, 2], modifications of the parton distribution functions of the proton inside a nucleus, is a particularly well studied example where $\mathcal{O}(10\%)$ effects are observed. Similarly, Gamow-Teller transitions of nuclei occur at rates that indicate that the axial coupling of the nucleon is modified at an even more significant level in medium-mass nuclei, being as large as a 30% effect in some cases [3, 4]. It is natural that such effects arise as a result of the strong dynamics that exist inside the nucleus. However, theoretically such effects are not understood in a compelling, predictive way and it is a contemporary challenge to provide a rigorous description of these effects using methods that are directly connected to the underlying theory of the strong interactions, Quantum Chromodynamics (QCD). This is not purely an academic exercise in understanding the structure of a nucleus; nuclei are becoming increasingly important as targets in contemporary and planned studies of neutrino properties and in many searches for physics beyond the Standard Model. The ability of the Long Baseline Neutrino Facility and other proposed neutrino experiments to determine the neutrino mass hierarchy and extract the CP violating phases in the neutrino mixing matrix is limited by neutrino flux and energy measurements on nuclear targets [5, 6]. These, in turn, are fundamentally limited by the current uncertainties in our knowledge of the axial (and induced pseudoscalar) form factors of nuclei. In many dark matter direct detection experiments, nuclear recoils are the primary signal mechanism. Expected rates therefore depend not only on the dynamics of the dark sector, but also on the amplitudes for interactions of the target nuclei (Ar, Si, Ge, Xe,. . .) with the current that mediates the connection to the dark sector. For example, for a dark sector that couples to the Standard Model via a scalar mediator, the relevant Standard Model input is the nuclear target matrix element of the scalar quark bilinear current, the so-called sigma term of the nucleus [7, 8]. An understanding of nuclear effects in these classes of experiments at a quantitative level is required to maximise their impact and is thus an important goal for QCD practitioners over the coming decade.

In this work, we develop the theoretical framework necessary for the QCD exploration of external currents in particularly simple multi-hadron systems. As the only known method with which to calculate the properties of hadrons (including nuclei) in QCD from first principles is through lattice QCD (LQCD), it is expected that the requisite understanding will involve lattice calculations. However lattice calculations are performed in Euclidean space and in a finite volume by necessity, which restricts the physical (infinite-volume Minkowski space) information that can be extracted. It is important to understand what information is accessible in such calculations and how it can be extracted. In its fully generality, this is a very challenging task and to make progress, we will focus on the limiting case of perturbatively interacting spin-zero systems in our current analysis.

II. MULTI-BOSON SYSTEMS

Over the last few years, systems of many identical composite bosons have been extensively studied in lattice QCD with particular focus on states with the quantum numbers of many like-charged pions. Following the classic works of Lee, Huang and Yang [9, 10], the theoretical understanding of the dependence of the ground state spectrum of these systems on the finite volume used in numerical calculations was developed in Refs. [11, 12]. There, the ground-state energy of n identical bosons of mass M in a cubic box of side length L was determined using time-ordered perturbation theory, with a Hamiltonian density of the form

$$\begin{aligned} H \;=\; & \sum_{\mathbf{k}} h^\dagger_{\mathbf{k}}\, h_{\mathbf{k}} \left(\frac{|\mathbf{k}|^2}{2M} - \frac{|\mathbf{k}|^4}{8M^3} \right) \\ & + \frac{1}{(2!)^2} \sum_{\mathbf{Q},\mathbf{k},\mathbf{p}} h^\dagger_{\frac{\mathbf{Q}}{2}+\mathbf{k}} h^\dagger_{\frac{\mathbf{Q}}{2}-\mathbf{k}}\, h_{\frac{\mathbf{Q}}{2}+\mathbf{p}}\, h_{\frac{\mathbf{Q}}{2}-\mathbf{p}} \left(\frac{4\pi a}{M} + \frac{\pi a}{M} \left(ar - \frac{1}{2M^2} \right) \left(|\mathbf{k}|^2 + |\mathbf{p}|^2 \right) \right) \\ & + \frac{\eta_3(\mu)}{(3!)^2} \sum_{\mathbf{Q},\mathbf{k},\mathbf{p},\mathbf{r},\mathbf{s}} h^\dagger_{\frac{\mathbf{Q}}{3}+\mathbf{k}} h^\dagger_{\frac{\mathbf{Q}}{3}+\mathbf{p}}\, h^\dagger_{\frac{\mathbf{Q}}{3}-\mathbf{k}-\mathbf{p}}\, h_{\frac{\mathbf{Q}}{3}+\mathbf{r}} h_{\frac{\mathbf{Q}}{3}+\mathbf{s}}\, h_{\frac{\mathbf{Q}}{3}-\mathbf{r}-\mathbf{s}} \,, \end{aligned} \tag{1}$$

where the operator $h_{\mathbf{k}}$ annihilates a boson with momentum $\mathbf{k}$ with unit amplitude, and terms are kept that will contribute at the order in the large-volume expansion to which we work. The momentum labels on the creation and annihilation operators are constrained such that three-momentum is conserved. The couplings a, r and $\eta_3(\mu)$ correspond to the two-particle scattering length and effective range, and to the leading momentum-independent three particle interaction.[1] In particular, the shift in the ground-state energy from n free bosons was determined to be

$$\Delta E_0(n,L) \;=\; \frac{4\pi\, a}{M\, L^3}\binom{n}{2}\left\{1-\left(\frac{a}{\pi\, L}\right)\mathcal{I}+\left(\frac{a}{\pi\, L}\right)^2\left[\mathcal{I}^2+(2n-5)\mathcal{J}\right]\right. \tag{2}$$
$$\left.-\left(\frac{a}{\pi\, L}\right)^3\left[\mathcal{I}^3+(2n-7)\mathcal{I}\mathcal{J}+\left(5n^2-41n+63\right)\mathcal{K}\right]\right\}+\binom{n}{2}\frac{8\pi^2a^3r}{M\, L^6}$$
$$+\binom{n}{3}\frac{1}{L^6}\left[\eta_3(\mu)\;+\;\frac{64\pi a^4}{M}\left(3\sqrt{3}-4\pi\right)\,\log\left(\mu L\right)\;-\;\frac{96a^4}{\pi^2 M}\,\mathcal{S}\right]\;+\;\mathcal{O}\left(L^{-7}\right)\,,$$

where μ is a renormalisation scale and

$$\mathcal{I} \;=\; -8.9136329\,,\qquad \mathcal{J}\;=\;16.532316\,,\qquad \mathcal{K}\;=\;8.4019240\,,\qquad \mathcal{S}_{\rm MS}\;=\;-185.12506\,,$$

are geometric constants arising from finite-volume loop contributions [11, 12]. The corresponding expression including $\mathcal{O}(1/L^7)$ corrections is presented in Ref. [12].

Determinations of the corresponding energy shifts in many-boson systems can be used to determine the various interactions in Eq. (1) for a given set of systems. To this end, sophisticated techniques have been constructed in order to study these complicated systems numerically in QCD [13–15]. Calculations using these methods have led to extractions of the $I=2$ two-pion interaction, the $I=3$ three-pion interaction and of the effects of these systems on other hadronic quantities [16, 17]. Using relations between baryons and mesons in QCD with $N_c=2$ colours, these results have also enabled a recent study of the analogues of nuclei for $N_c=2$ [18].

From considerations of chiral dynamics, QCD inequalities [19], and from the explicit numerical explorations mentioned above, it is apparent that interactions in isospin $I=n$ many-π^+ systems are repulsive and that there are no bound states for any n. Chiral symmetry guarantees that the strength of the interactions is perturbatively weak, so an expansion in the couplings a, r and $\eta_3(\mu)$ is expected to be reliable provided na/L remains small, as do similar combinations of the other couplings. Such systems therefore provide an ideal situation for the application of the methods discussed herein.

[1] The three-particle interaction $\eta_3(\mu)$ as defined in the Hamiltonian depends on the regularisation and renormalisation prescription as discussed in Ref. [11], but will not contribute at the order we work in this current study.

III. MATRIX ELEMENTS OF EXTERNAL CURRENTS IN MULTI-BOSON SYSTEMS

The time-ordered perturbation theory methods used to derive the energy shifts in Refs. [11, 12] order by order in the coupling and large-volume expansion also determine the state vector as an expansion in couplings (see, for example Ref. [20]). In particular, the n boson state can be expanded as

$$|n\rangle(a, r, \eta_3(\mu)) = |n^{(0)}\rangle + \eta|n^{(1)}\rangle + \eta^2|n^{(2)}\rangle + \eta^3|n^{(3)}\rangle + \ldots, \tag{3}$$

where $|n^{(0)}\rangle$ corresponds to the free n-particle system and subsequent terms are induced by perturbative interactions amongst the particles in the periodic volume. In the above expression, η is representative of any one of the couplings. Knowing the state vector, it is thus a simple matter to compute the expectation values of currents that are of phenomenological interest. To be general, we do not assume a particular type of current and consider the current density

$$J = \sum_{\mathbf{k}} \alpha_1 h^\dagger_{\mathbf{k}} h_{\mathbf{k}} + \sum_{\mathbf{k},\mathbf{Q},\mathbf{p}} \alpha_2 h^\dagger_{\frac{\mathbf{Q}}{2}+\mathbf{k}} h^\dagger_{\frac{\mathbf{Q}}{2}-\mathbf{k}}\ h_{\frac{\mathbf{Q}}{2}+\mathbf{p}}\ h_{\frac{\mathbf{Q}}{2}-\mathbf{p}}\,, \tag{4}$$

where α_1 and α_2 are constants that describe the momentum independent one-boson current and the two-boson current, respectively. The momentum sums on the two-body operator fix the total momentum $\mathbf{Q}$ in the initial and final state (the current does not transfer momentum), but allow for different relative momenta before and after the interaction with the current, $\mathbf{p}$ and $\mathbf{k}$, respectively. The particular strengths of the different terms, and the flavour and spin dependence of the interactions may differ for different fundamental currents, but the above form is general up to momentum-dependent and higher-body corrections that are suppressed by additional powers of $1/L$ in our results. For simplicity, we have assumed the soft limit in which the current does not inject momentum into the system so that the two-hadron current amounts to a simple reshuffling of the boson momenta. No obstacles are encountered in the extending the current results to the case of momentum transfer provided it is small compared to the hadronic scale.

The full finite volume matrix elements of J involve the various terms in Eq. (3). The calculation is straightforward (if a little tedious) and the reader is referred to Refs. [11, 12] for more details; we will only state the result. The matrix elements of J for systems of n pions up to $O(L^{-5})$ are as follows:

$$
\begin{aligned}
L^3 \langle n|J|n\rangle \;=\; & n\alpha_1 + \frac{n\alpha_1 a^2}{\pi^2 L^2}\binom{n}{2}\mathcal{J} + \frac{\alpha_2}{L^3}\binom{n}{2} \\
& + \frac{2n\alpha_1 a^3}{\pi^3 L^3}\binom{n}{2}\left\{\mathcal{K}\binom{n}{2} - \left[\mathcal{I}\,\mathcal{J} + 4\mathcal{K}\binom{n-2}{1} + \mathcal{K}\binom{n-2}{2}\right]\right\} - \frac{2\alpha_2 a}{\pi L^4}\binom{n}{2}\mathcal{I} \\
& + \frac{n\alpha_1 a^4}{\pi^4 L^4}\Bigg[3\mathcal{I}^2\mathcal{J} + \mathcal{L}\left(186 - \frac{241n}{2} + \frac{29}{2}n^2\right) + \mathcal{J}^2\left(\frac{n^2}{4} + \frac{3n}{4} - \frac{7}{2}\right) \\
& \qquad + \mathcal{I}\,\mathcal{K}(4n-14) + 32\mathcal{U}(n-2) + 16\mathcal{V}(n-2)\Bigg] + \mathcal{O}(1/L^5)\,.
\end{aligned} \tag{5}
$$

Representative contributions for the various terms are shown in Fig. 1. This expression is the primary result of the current work and has been calculated through to the second order at which the two-boson current contributes so that the consistency of an extraction can be checked between orders. The additional numerical constants that enter this expression are

$$
\mathcal{L} = 6.9458079, \qquad \mathcal{U} = 85.1269266, \qquad \mathcal{V} = -64.1765107\,,
$$

and the sums which lead to these values are defined by

$$
\mathcal{L} \;=\; \sum_{\vec{i}\neq 0} \frac{1}{|\vec{i}|^8}\,, \tag{6}
$$

$$
\mathcal{U} \;=\; \sum_{\vec{i},\vec{j}\neq 0} \frac{1}{|\vec{i}|^4|\vec{j}|^2\left(|\vec{i}|^2+|\vec{j}|^2+|\vec{i}+\vec{j}|^2\right)} + \sum_{\vec{i},\vec{j}\neq 0} \frac{1}{|\vec{i}|^2|\vec{j}|^2\left(|\vec{i}|^2+|\vec{j}|^2+|\vec{i}+j|^2\right)^2}\,, \tag{7}
$$

$$
\mathcal{V} \;=\; \sum_{\vec{i}\neq 0,\vec{j}} \frac{1}{|\vec{i}|^6\left(|\vec{i}|^2+|\vec{j}|^2+|\vec{i}+\vec{j}|^2\right)} + \sum_{\vec{i}\neq 0,\vec{j}} \frac{1}{|\vec{i}|^4\left(|\vec{i}|^2+|\vec{j}|^2+|\vec{i}+\vec{j}|^2\right)^2}\,, \tag{8}
$$

where $\vec{i}$ and $\vec{j}$ are three-tuples with integer valued components. These three- and six-dimensional sums are convergent and can be computed with the use of the Poisson summation formula, yielding the values above.

From the above expression, we see that the finite-volume matrix elements only depend on the one-boson current, α_1, at leading order and at next-to-leading order in the large volume perturbative expansion. Dependence on the two-boson current coupling, α_2, arises at $\mathcal{O}([\frac{a}{\pi L}]^3)$; for a repulsive interaction such weak sensitivity is expected. Notice that neither r or $\eta_3(\mu)$ enter the calculation at $\mathcal{O}(1/L^4)$ however they will contribute at higher orders in $1/L$. Similarly, a three-boson contribution to the current will eventually be relevant. As with the energy levels in Eq. (2), off-shell effects will lead to additional exponentially suppressed volume dependence $\sim \exp(-M_\pi L)$ where M_π is the pion mass which dominates such effects as the pion is the lightest hadronic state.

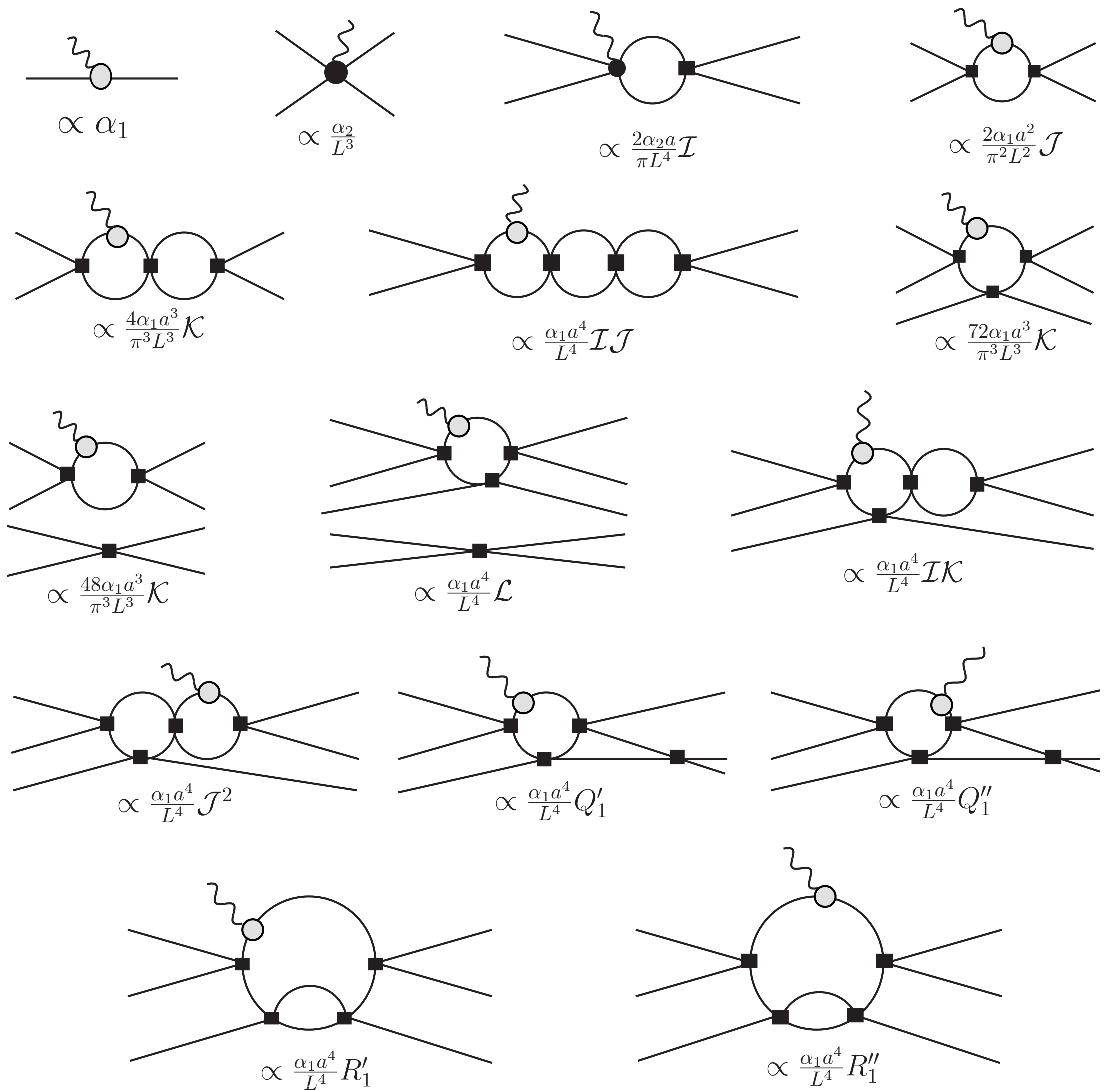

FIG. 1: Representative contributions in the calculation of the finite volume matrix elements. The solid lines correspond to the boson propagators and the vertices indicate either strong scattering (dark square) or one- and two-body currents (light and dark circles, respectively). The contribution of a given topology is shown up to combinatoric factors. The combinations $\mathcal{U} = Q_1' + Q_1''$ and $\mathcal{V} = R_1' + R_1''$ are used in the final expression.

IV. DISCUSSION

The result presented above provides the expected hadronic behaviour of a multi-boson matrix element of a local (at the hadronic scale) operator in a finite volume. It explicitly depends on the one-body and two-body couplings of the hadrons to the current and also on the two-body interactions between the hadrons (higher body interactions will become relevant for sub-leading terms in the volume expansion). Lattice QCD calculations of the corresponding matrix elements in systems of n spin-zero bosons can be matched onto these expressions to determine the external current interactions in the appropriate hadronic theory once the two-boson interaction is determined from the shifts in energies of n-boson systems in a finite volume. Consequently, the results derived herein will be useful in the analysis of lattice QCD calculations of matrix elements of currents in weakly-interacting multi-pion states such as those presented in preliminary form in Ref. [21].

Our calculation has focused on the case of identical spin zero bosons with perturbatively weak interactions at energies near threshold in the appropriate channels. The inclusion of the effects of angular momentum and spin degrees of freedom, and of more complicated systems with coupled channels is left for future study. Further work is also necessary to understand the behaviour of multi-hadron matrix elements with non-perturbatively strong interactions or when the expansion in a/L breaks down. For two particles, the non-perturbative dependence of the ground state energy on the spatial extent of a periodic volume has been known for many years [22, 23] and there has been significant recent progress [24–26] toward achieving the same level of understanding for three-particle systems. The effects of finite volume on $1 \to 2$ particle transitions induced by an external current have also been understood for simple cases in the pioneering work of Lellouch and Lüscher [27] and recently generalised to more complicated cases in Refs. [28–33]. It seems likely that the approaches used in these analyses could be extended to consideration of $2 \to 2$ current matrix elements and perhaps to the three-particle case. For strongly interacting systems with more than three particles, new methods are required to have analytic control over the interactions of multi-hadron systems and over the relation between multi-hadron matrix elements in QCD and in the hadronic theory. In the absence of such advances, the matching between QCD calculations of matrix elements in finite volume and those in the hadronic effective theory can be implemented through numerical calculations of correlators in the hadronic theory in a finite volume for varying input low-energy constants (the analogues of the current couplings α_1 and α_2) until the QCD results are reproduced, thereby determining the hadronic couplings.

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