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Comment on "Are two nucleons bound in lattice QCD for heavy quark masses? - Sanity check with Lüscher's finite volume formula -"

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In this comment, we address a number of erroneous discussions and conclusions presented in the recent preprint arXiv:1703.07210. In particular, we show that lattice QCD determinations of bound states at quark masses corresponding to a pion mass of $m_\pi = 806$ MeV are robust, and that the extracted phases shifts for these systems pass all of the "sanity checks" introduced in arXiv:1703.07210.

In the last decade, significant progress has been made in the study of multi-hadron systems using lattice QCD, with the first calculations of multi-baryon bound states and their electroweak properties and decays having been performed [1–18]. It is imperative that the methods used in these calculations be robust; investigations such as those of the HALQCD collaboration in arXiv:1703.07210 (henceforth referred to as HAL) are vital provided they are carried out correctly. However, as we show in detail, HAL contains a number of major errors that invalidate its conclusions. Since we have recently refined one of the analyses that is criticised in HAL, we focus our attention on the conclusions drawn regarding this case in particular.

The central point addressed by HAL is whether there exist bound states in the $^1S_0$ and $^3S_1$ two-nucleon channels at heavy quark masses. Three independent groups have analysed lattice QCD calculations at quark masses corresponding to a heavy pion mass of ~ 800 MeV (one set of calculations used quenched QCD) and found that there are bound states in these channels. Each of these groups has concluded this by extracting energies from two-point correlation functions with the quantum numbers of interest at two or more lattice volumes and demonstrating, through extrapolations based on the finite-volume formalism of Lüscher [19, 20], that these energies correspond to an infinite-volume state that is below the two-particle threshold and is hence a bound state. Each group has used different technical approaches, and all are in reasonable agreement given the uncertainties that are reported. The HALQCD group has also investigated these two-particle channels using a method (also based on the work of Lüscher [19, 21]) that involves constructing Bethe-Salpeter wavefunctions, but do not find evidence for bound states in these channels.[1] We

[1] In the $\Lambda\Lambda$ channel, the HALQCD approach does indicate a bound state, but the binding energy is found to be significantly different from that determined by examining of finite-volume energy levels [6].

note, however, that recent incarnations of the HALQCD method introduce unquantified systematic effects (see Refs. [22–24] and the nuclear physics overview talks in recent proceedings of the International Symposium on Lattice Field Theory [25–27]). Here, we focus our criticisms of HAL on several specific points.

1. Misinterpretation of energies and source independence

Fig. 2 of HAL contains a compilation of results for the ground states of the $^1S_0$ and $^3S_1$ two-nucleon channels. Unfortunately the figure includes a second state from Ref. [14] that the authors of Ref. [14] explicitly indicate is not the ground state, and reporting it as such is a critical error on which many of the invalid arguments of HAL are based.[2] There is a small scatter in the remaining results that is due to statistical fluctuations, discretisation artifacts and exponentially-small residual finite-volume effects, but, taken as a whole, there is no inconsistency in these results. In addition, a further recent study of axial-current matrix elements using a different set of interpolators [18] also finds a consistent negatively-shifted energy on the $32^3 \times 48$ ensemble used in this comparison. Fig. 2 in HAL also fails to include the energies extracted in Ref. [6] on the largest volume, which crucially dominate the extraction of the binding energy. Without the results from this large volume, the confidence in the binding energy in Ref. [6] would be significantly diminished. It is therefore vital that this information be included in any discussion of these results. Fig. 1 below shows a corrected summary of the energy levels extracted for the ground states of the $^1S_0$ and $^3S_1$ two-nucleon systems in different volumes in the literature at this particular quark mass. No significant interpolator dependence is observed, as is indicated by simple fits to the reported results for each volume, with all these fits having acceptable values of χ^2 per degree of freedom. Fig. 13 of HAL is also erroneously described as indicating that scattering state results are not source independent. The results show three energy levels where different interpolating operators are consistent within one standard deviation, and one energy level that differs at two standard deviations. This signals broad agreement within the reported uncertainties and is not a sound statistical basis for a claim of inconsistency.

In summary, comparison of results from the different interpolators in Refs. [6, 7, 14, 18] shows that both bound and scattering-state energy levels are source-independent within reported uncertainties. The claims to the contrary in HAL are baseless.

2. Volume scaling of energies

The authors of HAL claim that the single-exponential behaviour found in our work, Refs. [6, 7], and in that of Ref. [14], is a "mirage" arising from the cancellation of two or more energy eigenstates contributing to the correlation functions with opposite signs. This interpretation of the negatively-shifted states in these works is exceedingly unlikely, however, as it would need to occur in an almost identical way for multiple different volumes. For each of the different analyses of the 806 MeV ensembles in Fig. 1 (NPLQCD2013 $d = 0$, NPLQCD2013 $d = 2$ and Berkowitz2016 $d = 0$), identical sources and sinks were used in each of three volumes (two volumes in the case of Berkowitz2016). Scattering-state eigenenergies necessarily change significantly with volume, having power-law dependence as dictated by the Lüscher quantisation condition. While it is possible that, in a given volume, a correlator for a particular source-sink interpolator combination could

[2] Whether the quoted value for the second energy in Ref. [14] is a true estimate of an excited-state energy is a question for future discussion. However for the ground states, all results unambiguously agree.

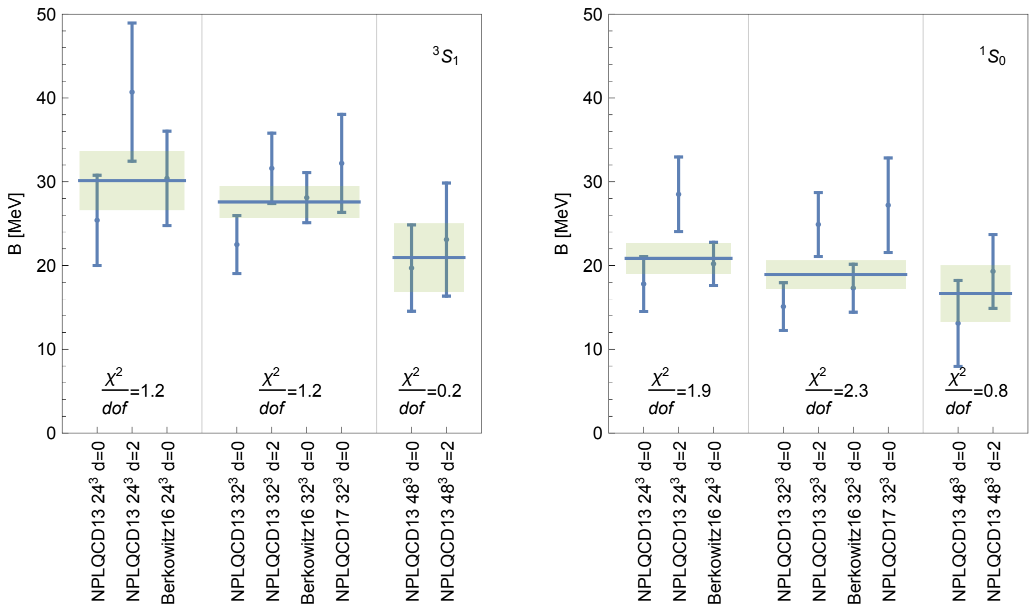

FIG. 1: Binding energies for the $^3S_1$ and $^1S_0$ ground states at $m_\pi = 806$ MeV found in the literature: NPLQCD13 [6], Berkowitz16 [14], and NPLQCD17 [18] ($d = 0$ and $d = 2$ refer to the magnitude of the centre-of-mass momentum used in the calculations in units of $2\pi/L$). The three regions in each panel correspond to three different volumes: $L = 24$, 32, and 48 from left to right. Uncertainties listed in the original references are combined in quadrature. The horizontal lines and shaded bands represent the central value and one standard deviation bands on fits to the indicated data, respectively.

exhibit a cancellation between contributions of two scattering states that produces an energy level below threshold, it is very unlikely that the cancellation would persist in different volumes as the scattering-state eigenenergies change significantly with volume. As shown in Fig. 2, for example, the volume-independent interpolators used in Ref. [6, 7] produce energy levels in the three different volumes that are statistically indistinguishable, and even the approach to single-exponential behaviour does not depend on volume. The figure shows the effective masses of the smeared-point correlation functions, but the same features are seen in all other source-sink interpolator combinations that are studied. This rules out the possibility that the negatively-shifted signals are caused by cancellations between scattering states. The third very large volume used in our works [6, 7] makes this an extremely robust statement as the spatial volumes from which we draw these conclusions vary by a factor of eight.

3. Consistency of Effective Range Expansion ("HAL Sanity Check (i)")

If the effective range expansion (ERE) is a valid parametrization of the scattering amplitude at low energies, the analyticity of the amplitude as a function of the centre-of-mass energy implies that the ERE obtained from states with positively-shifted energies ($k^{*2} > 0$, where k^* is the centre-of-mass interaction momentum) must be consistent with that obtained from states with negatively-shifted energies ($k^{*2} < 0$). Although HAL finds that the NPLQCD results pass this test, we demonstrate how robust the results in Refs. [6, 7] are in this regard through the plots presented in Fig. 3. This figure shows fits to the ERE using both ground states ($n = 1$) and first excited states ($n = 2$) (color-filled bands). These are overlaid on ERE fits using only the

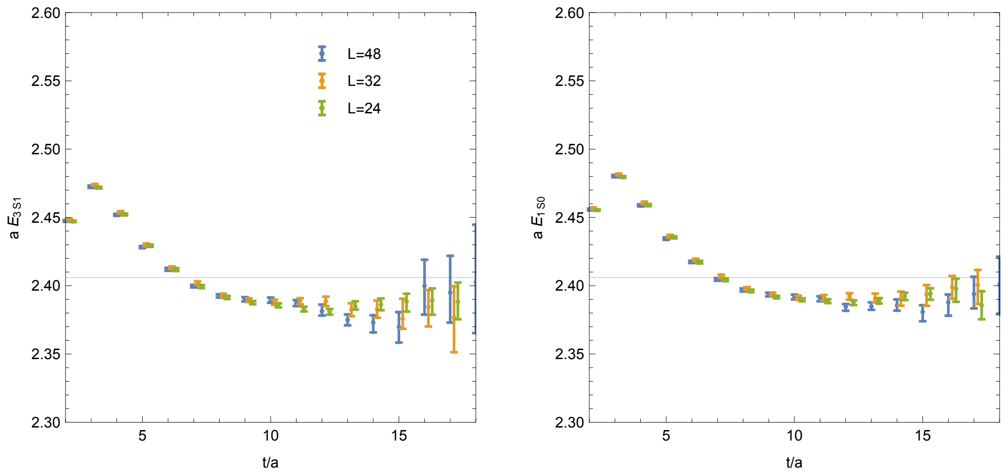

FIG. 2: The effective mass plots associated with the $d = 0$ smeared-point correlators in the $L = 24$, 32, and 48 ensembles of Ref. [6, 7]. The left(right) panel shows the ${}^3S_1({}^1S_0)$ channel. Quantities are expressed in lattice units. The horizontal grey line marks the infinite-volume energy of two non-interacting nucleons.

ground states (hashed bands). The two sets of bands are fully consistent with each other, proving that this check is unambiguously passed. The same feature is seen for three-parameter ERE fits, with significantly larger uncertainty bands. The difference in the size of uncertainties in the phase shift between the fits with and without the $n = 2$ data shows that conclusions about the behaviour and/or validity of the ERE for datasets only near the bound-state pole are likely subject to significant uncertainties. We also note that it is entirely possible that scattering phase shifts at large quark masses can only be described by a linear truncation of the ERE in a region very close to $k^{*2} = 0$, so failing such a check does not allow any conclusion about the reliability of the extracted energy levels to be drawn. Indeed, it is known that in nature, the effective range expansion of the ${}^3S_1$ phase shift around $k^{*2} = 0$ and around the deuteron pole are different (albeit slightly) [28].

4. Residue of the S-matrix at the bound-state pole ("HAL Sanity check (iii)")

The sign of the residue of the S-matrix at the bound-state pole is fixed. This requirement leads to the following condition on $k^* \cot\delta$:

$$\frac{d}{dk^{*2}}(k^* \cot\delta + \sqrt{-k^{*2}})\Big|_{k^{*2}=-\kappa^{(\infty)2}} < 0, \tag{1}$$

where $\kappa^{(\infty)}$ is the infinite-volume binding momentum. As is seen from Fig. 4, which shows the results of Refs. [6, 7], the slope of the two-parameter ERE fit to the $k^* \cot\delta$ function (color-filled bands) in all channels is never greater than the slope of $-\sqrt{-k^{*2}}$ (grey bands) at the corresponding bound-state pole. The uncertainty in the tangent line to the $-\sqrt{-k^{*2}}$ function at $k^{*2} = -\kappa^{(\infty)2}$ arises from the uncertainty in the values of $\kappa^{(\infty)}$ (further discussion of this will be presented in a forthcoming article [29]). A similar conclusion can be drawn from three-parameter ERE fits. Thus the results of Refs. [6, 7] pass this check, in stark contrast to the claims of HAL.

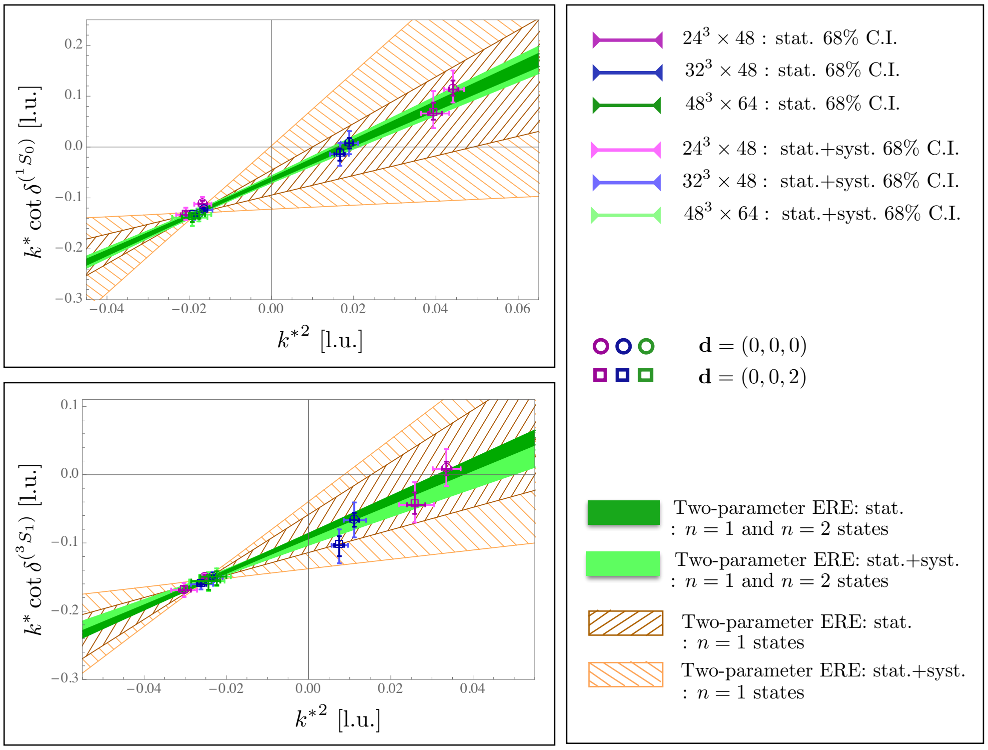

FIG. 3: $k^* \cot\delta$ vs. the square of the centre-of-mass momentum of two baryons, k^{*2}, along with the bands representing fits to two-parameter EREs obtained from i) only the ground states ($n = 1$) and ii) from both the ground states ($n = 1$) and the first excited states ($n = 2$). The plots show the consistency of the ERE between negative and positive k^{*2} regions in both the $^1S_0$ and $^3S_1$ channels. Quantities are expressed in lattice units (l.u.).

Discussion

Given the discussion above, the NPLQCD results presented in the "NPL2013" row of Table IV of HAL, reproduced below,

	$NN(^1S_0)$				$NN(^3S_1)$			
Data	Source independence	Sanity check (i)	(ii)	(iii)	Source independence	Sanity check (i)	(ii)	(iii)
NPL2013 [27,28]	No			No	No			No

should be replaced by

	$NN(^1S_0)$				$NN(^3S_1)$			
Data	Source independence	Sanity check (i)	(ii)	(iii)	Source independence	Sanity check (i)	(ii)	(iii)
NPL2013 [27,28]	Yes	Passed	Passed	Passed	Yes	Passed	Passed	Passed

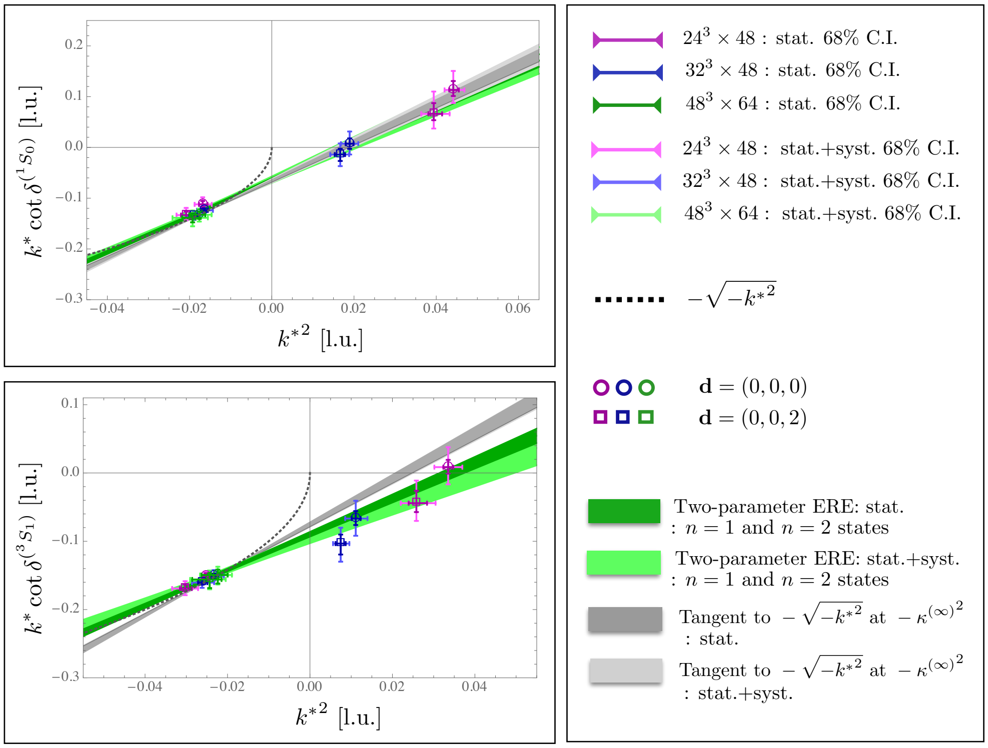

FIG. 4: The two-parameter ERE is compared with the tangents to the $(-\sqrt{-k^{*2}})$ curve at values of $k^{*2} = -\kappa^{(\infty)2}$. The plots show that all the identified energy eigenstates in this work are consistent with the criterion in Eq. (1) within uncertainties. Quantities are expressed in lattice units (l.u.).

where we have taken the liberty of changing the notation used to indicate passing a "sanity check" in HAL from a blank entry to "Passed". The major inconsistencies found in this row of the table suggest that the conclusions reached as a whole in HAL should be viewed with extreme caution. We are currently revisiting the other NPLQCD analyses discussed in HAL. Ref. [30] refutes the HAL criticisms of source-dependence leveled at the works of the PACS-CS collaboration [9], and Ref. [27] by one of the current authors provides a summary of the evidence for the validity of ground-state identifications in two-nucleon systems.

The incorrect conclusions reached in HAL potentially arise from attempting to reanalyse highly correlated data, such as those encountered in the phase-shift analyses, without making use of those correlations. Given the robustness of the existence of bound states in the two-nucleon channels at $m_\pi = 806$ MeV, the authors of HAL would do well to investigate the uncontrolled systematics in the HALQCD approach that have been previously discussed [22–27].

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