Finite-volume corrections to charge radii

J. M. M. Hall\textsuperscript{a}, D. B. Leinweber\textsuperscript{a}, B. J. Owen\textsuperscript{a}, R. D. Young\textsuperscript{ab}

\textsuperscript{a}Special Research Centre for the Subatomic Structure of Matter (CSSM), School of Chemistry and Physics, University of Adelaide 5005, Australia
\textsuperscript{b}ARC Centre of Excellence for Particle Physics at the Terascale (CoEPP), School of Chemistry and Physics, University of Adelaide 5005, Australia

Abstract

The finite-volume nature of lattice QCD entails a variety of effects that must be handled in the process of performing chiral extrapolations. Since the pion cloud that surrounds hadrons becomes distorted in a finite volume, hadronic observables must be corrected before one can compare with the experimental values. The electric charge radius of the nucleon is of particular interest when considering the implementation of finite-volume corrections. It is common practice in the literature to transform electric form factors from the lattice into charge radii prior to analysis. However, there is a fundamental difficulty with using these charge radii in a finite-volume extrapolation. The subtleties are a consequence of the absence of a continuous derivative on the lattice. A procedure is outlined for handling such finite-volume corrections, which must be applied directly to the electric form factors themselves rather than to the charge radii.

Keywords:
electric charge radii, effective field theory, finite-volume corrections, lattice QCD

1. Introduction

Lattice QCD provides important non-perturbative techniques for the analysis of many observables. One of the notable features of lattice QCD is that it must be performed in a finite volume. The associated finite-volume effects can be used to access interesting phenomena. For example, multi-hadron states are only resolvable at finite lattice sizes; the discrete energy eigenvalues become increasingly close together as the box size becomes large. The finite-volume nature of lattice QCD has important consequences, some of which require careful attention. For example, although regularization in both the infrared and ultraviolet regions is an automatic feature of lattice QCD with a finite lattice spacing,
finite-sized phenomena, such as the virtual pion clouds that surround hadrons, become distorted. This results in deviations in the values of lattice observables that can become significant in the chiral regime \([1, 2, 3, 4, 5, 6]\). Therefore, a method for correcting finite-volume effects by estimating their size is sought, using a complementary approach, such as chiral effective field theory (\(\chi\text{EFT})\) \([3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13]\).

Study of the quark mass dependence of lattice QCD simulation results can be particularly insightful for examining the chiral properties of hadrons. In relating lattice calculations to experimental results, it is essential to incorporate the low-energy features of QCD in order to obtain reliable extrapolations in both quark mass and volume.

In lattice QCD, form factors are measured at discrete values of momentum transfer, corresponding to the quantization of the momentum modes on the finite spatial volume \([10, 11, 14, 15, 16, 17, 18, 19, 20, 21, 22]\). Once form factors have been extracted from lattice simulations, they are typically converted directly into charge radii. The essential difficulty lies in the definition of the charge ‘radius’ at finite volume (more precisely, the slope of the form factor at zero momentum transfer, \(Q^2 = \vec{q}^2 - q_0^2\)). In order to define the radius, a derivative must be applied to the electric form factor, with respect to a small momentum transfer. This approach breaks down on the lattice, where only discrete momentum values are allowed.

In most cases, calculating the finite-volume corrections poses no essential problems \([5, 13, 6, 23, 24, 25, 26]\). However, because of the absence of a continuous derivative on the lattice, the treatment of the electric charge radius is more subtle \([9, 27, 28]\). Therefore, a method is outlined for handling finite-volume corrections to a given lattice simulation result.

Finite-volume charge radii are calculated using the finite-volume electric form factors, \(G_{EL}(Q^2)\), with \(Q^2\) taking an allowed value on the lattice. It will be shown that the finite-volume corrections to the loop integrals must be applied before the conversion from the form factor to the charge radius. An extrapolation in \(Q^2\) is then chosen in order to construct an infinite-volume charge radius, defined in the usual manner.

2. Effective field theory

In heavy-baryon chiral perturbation theory (\(\chi\text{PT})\), it is usual to define the Sachs electromagnetic form factors, \(G_{E,M}\), which parametrize the matrix element
for the quark current, \(J_\mu\), as

\[
\langle B(p')|J_\mu|B(p)\rangle = \bar{u}^{(p')}(p') \left\{ v_\mu G_E(Q^2) + \frac{i\epsilon_{\mu\nu\rho\sigma} S^\nu v^\rho q^\sigma}{m_B} G_M(Q^2) \right\} u^{(p)}(p),
\]

(1)

where \(v\) is the velocity of the baryon and \(Q^2 = -q^2 = -(p' - p)^2\). Lattice QCD results are often constructed from an alternative representation, using the form factors \(F_1\) and \(F_2\), which are called the Dirac and Pauli form factors, respectively. The Sachs form factors are simply linear combinations of \(F_1\) and \(F_2\)

\[
G_E(Q^2) = F_1(Q^2) - \frac{Q^2}{4m_B^2} F_2(Q^2),
\]

(2)

\[
G_M(Q^2) = F_1(Q^2) + F_2(Q^2).
\]

(3)

In the heavy-baryon formulation of Eq. (1), the spin operator, \(S_\mu v = -\frac{1}{8}\gamma_5[\gamma_\mu, \gamma_\nu]v_\nu\), is used [29, 30]. The momentum transfer dependence in the electric form factor, \(G_E(Q^2)\), allows a charge radius to be defined in the usual manner

\[
\langle r^2\rangle_E = \lim_{Q^2 \to 0} -6\frac{\partial G_E(Q^2)}{\partial Q^2}.
\]

(4)

2.1. Loop integral definitions

The loop integrals, in the continuum limit, that contribute to the electric form factor of the nucleon are invariant under arbitrary translations of the internal momentum \(\vec{k} \to \vec{k} + \delta\vec{k}\). However, a finite-volume sum over discrete loop momenta is only invariant if \(\delta\vec{k}\) is an allowed value of momentum on the lattice. The loop integrals in the heavy-baryon approximation that correspond to the leading-order diagrams in Figs. [1] through [5] are obtained by performing the pole integration for \(k_0\)

\[
\mathcal{T}_N(q^2) = \frac{\chi_N}{3\pi} \int d^3k \frac{(k^2 - \vec{k} \cdot \vec{q})}{\omega_k \omega_{k-q}(\omega_k + \omega_{k-q})},
\]

(5)

\[
\mathcal{T}_\Lambda(q^2) = \frac{\chi_\Lambda}{3\pi} \int d^3k \frac{(k^2 - \vec{k} \cdot \vec{q})}{(\omega_k + \Delta)(\omega_{k-q} + \Delta)(\omega_k + \omega_{k-q})},
\]

(6)

\[
\mathcal{T}_{\text{tad}}(q^2) = \frac{\chi_t}{\pi} \int d^3k \frac{1}{\omega_k + \omega_{k-q}},
\]

(7)
where \( \omega \vec{k} = \sqrt{\vec{k}^2 + m^2} \), \( m \) is the pion mass, and \( \Delta \) is the Delta-nucleon mass-splitting. Note that each integral does not explicitly depend on \( Q^2 \), but depends on the three-momentum transfer squared, \( \vec{q}^2 \). The chiral coefficients \( \chi_N, \chi_\Delta \) and \( \chi_t \) are derived from couplings arising in the Lagrangian of chiral perturbation theory [31].

\[
\chi_N^{\text{prot}} = \frac{5}{16\pi^2 f_\pi^2} (D + F)^2 = -\chi_N^{\text{neut}}, \tag{8}
\]

\[
\chi_\Delta^{\text{prot}} = \frac{5}{16\pi^2 f_\pi^2} \frac{4C^2}{9} = -\chi_\Delta^{\text{neut}}, \tag{9}
\]

\[
\chi_t^{\text{prot}} = \frac{1}{16\pi^2 f_\pi^2} = -\chi_t^{\text{neut}}, \tag{10}
\]

where the value of the pion decay constant is \( f_\pi = 92.4 \text{ MeV} \). The values for the couplings are estimated from the SU(6) flavor-symmetry relations [30, 32] and from phenomenology: \( D = 0.76, F = \frac{5}{4}D \) and \( C = -2D \).

To obtain the integrals that allow the determination of the quark mass expansion of the electric charge radius, one takes the derivative of each infinite-volume integral, \( T(\vec{q}^2) \), with respect to momentum transfer, \( \vec{q}^2 \), as \( \vec{q}^2 \to 0 \):

\[
T = \lim_{\vec{q}^2 \to 0} -6 \frac{\partial T(\vec{q}^2)}{\partial \vec{q}^2}. \tag{11}
\]

This derivative is equivalent to that of Eq. (4) in the Breit frame, defined by zero energy transfer to the nucleon \( (\vec{q}^\mu = (0, \vec{q})) \). Using the derivative forms, \( T \), therefore allows one to recover the familiar chiral expressions for the quark mass dependence of the charge radii.

2.2. Finite-volume corrections

In the analysis of finite-volume effects within \( \chi \)EFT, one requires an evaluation of the correction associated with replacing the continuum loop integrals by finite sums. This correction is expressed in the form

\[
\delta_L[T] = \chi \left[ \frac{(2\pi)^3}{L_x L_y L_z} \sum_{k_x,k_y,k_z} \int d^3k \right] I, \tag{12}
\]

for an integrand, \( I \). This is not so straightforward in the case of the charge radius, which involves a \( \vec{q}^2 \) derivative. Because of the fact that only certain, discrete
Figure 1: The pion loop contributions to the electric charge radius of a nucleon. All charge conserving pion-nucleon transitions are implicit.

Figure 2: The pion loop contribution to the electric charge radius of a nucleon, allowing transitions to the nearby and strongly-coupled $\Delta$ baryons.

Figure 3: The tadpole contribution at $\mathcal{O}(m_q)$ to the electric charge radius of a nucleon.
values of momenta are allowed on the lattice, only a finite-difference equation may be constructed from these allowed momenta. The finite-difference equation, ideally, would be constructed from the lowest value of \( \vec{q}^2 \) available on the lattice, \( \vec{k}_{\text{min}}^2 = (2\pi \vec{n}/L)^2 \) (where \( \vec{n} \) is a lattice unit vector). This is not possible to do in the Breit frame, where the lowest \( \vec{q}^2 \) value is at least \( 2(2\pi \vec{n}/L)^2 \), which, on a moderate lattice size of 3 fm, is approximately \((0.58 \text{ GeV})^2\). In order to obtain a suitable estimate of the slope of the form factor at \( \vec{q}^2 = 0 \), a procedure is outlined for evaluating finite-volume corrections using the lowest available \( \vec{q}^2 \) value. Since the finite-volume corrections are applied directly to the form factor, an infinite-volume radius may be estimated. Thus, the quark mass behaviour of the radius may be examined independently of the finite-volume effects.

In order to illustrate the effect of using the loop integrals evaluated at allowed, and unallowed, values of momentum transfer, \( \vec{q}_i \) on the lattice, a comparison is shown in Figs. 4 and 5 in which the finite-volume correction to the one-pion loop integral (Eqs. (5) & (6)) is plotted as a function of box size, \( L \). In Fig. 4 the momentum transfer, \( \vec{q}_i \) is taken to be \( \vec{k}_{\text{min}} \). In evaluating the loop sums, a momentum translation of \( \delta \vec{k} = \vec{k}_{\text{min}}/2 \) is not an allowed value, and the finite-volume correction is inconsistent. This is a consequence of spoiling the continuous symmetry by the discretization of the momenta. In Fig. 5, \( \delta \vec{k} = \vec{k}_{\text{min}} \) is an allowed value, and the translated and untranslated results for the finite-volume correction are identical.

Note that it is possible to obtain a momentum transfer that is not a standard lattice vector by introducing twisted boundary conditions on the valence quark propagators. In tuning the twist angle to access non-integer momentum states, one must be careful to account for modified contributions to finite-volume corrections, as discussed in Ref. [28].

3. Procedure for obtaining charge radii at finite volume

In extracting radii from lattice simulations, one should start with the form factors as extracted from the lattice, and only convert them into radii (using a suitable Ansatz for the \( Q^2 \)-behaviour) after correcting for lattice finite-volume effects. The finite-volume correction to \( G_E(Q^2) \) is achieved by subtracting the difference between the sum and integral loop contributions, from Eq. (12)

\[
G_E(Q^2) = G_E^L(Q^2) - \delta_L[\mathcal{T}(\vec{q}^2)],
\]

where \( \mathcal{T} = \mathcal{T}_N + \mathcal{T}_\Delta + \mathcal{T}_{\text{tad}} \). In order to maintain conservation of charge, a subtraction of the finite-volume corrections at zero momentum transfer, \( \delta[\mathcal{T}(\vec{q}^2 = 0)] \), is
Figure 4: (color online). Finite-volume correction for the leading-order loop integrals contributing to $G_E$, with $\vec{q} = \vec{k}_{\text{min}}$. The choice of $\delta \vec{k} = \vec{k}_{\text{min}}/2$ is not an allowed value on the lattice. The momentum translated and untranslated behaviour of the finite-volume correction are inconsistent with each other.

Figure 5: (color online). Finite-volume correction for the leading-order loop integrals contributing to $G_E$, with $\vec{q} = \vec{k}_{\text{min}}$. The choice of $\delta \vec{k} = \vec{k}_{\text{min}}$ is an allowed value on the lattice. Therefore, the momentum translated and untranslated behaviour of the finite-volume correction are identical.
introduced

\[ \delta_L[T(\vec{q}^2)] \rightarrow \delta_L[T(\vec{q}^2)] - \delta_L[T(0)]. \]  

(14)

The second term of Eq. (14) ensures that both infinite- and finite-volume form factors are correctly normalized, i.e. \( G_E^L(0) = 1 = G_E(0) \), independent of the nucleon momentum. This normalization procedure assumes that charge conservation is satisfied in a finite volume, as demonstrated by the following numerical analysis. Within the framework of \( \chi \)EFT, preservation of the lattice Ward-Takahashi Identity in a finite volume has been addressed in Ref. [27].

A lattice QCD calculation was undertaken to demonstrate charge conservation in the rest frame, and in several boosted frames of increasing momenta. Using the temporal component of a conserved vector current, and the prescription outlined in Ref. [17], the Sachs electric form factor, \( G_E^L \), at zero momentum transfer, was calculated for external momenta: \( \vec{p} = \vec{0}, \vec{k}_{\text{min}}, 2 \vec{k}_{\text{min}} \) and \( 3 \vec{k}_{\text{min}} \), where \( \vec{k}_{\text{min}} \) is the minimum available three-momentum on the lattice. In all cases considered, the extracted value of \( G_E^L(Q^2 = 0) \) was consistent with unity up to the level of precision present in the propagators used in the calculation, indicating that charge conservation is satisfied.

In general, matrix elements in lattice QCD depend on the external momentum, as discussed in detail in Refs. [27, 28]. That is, the breaking of SO(4) symmetry entails a boost-dependence of the current matrix elements in a finite volume. In that case, the frame, and current component, must be specified in obtaining finite-volume corrections to the matrix elements calculated on the lattice. However, in the heavy-baryon approximation, the finite-volume corrections to the leading-order loop contributions (Figs. [1] through [3]) depend only on \( \vec{q}^2 \), and not on the boost of the initial or final nucleon state. Physically, this is simply a consequence of a lack of recoil energy-dependence in the intermediate nucleon propagator. This boost-invariance is also realized in Eq. (A1) of Ref. [28], by removing the twisted boundary condition and the partial quenching.

With the finite-volume corrected form factors at hand, the charge radii, \( \langle r^2 \rangle_E \), can be recovered from the form factors by using a suitable \( Q^2 \) parametrization. At large \( L \), and hence with numerous small \( Q^2 \) values, a formal \( Q^2 \)-expansion from \( \chi \)EFT would be ideal, such as that used in Ref. [33]. At smaller values of \( L \), with limited \( Q^2 \) values, it is common to work with a more phenomenological Ansatz, such as the dipole form

\[ G_E(Q^2_{\text{min}}) = \left( 1 + \frac{Q^2_{\text{min}} \langle r^2 \rangle_E}{12} \right)^{-2}, \]  

(15)
where $Q_{\text{min}}^2 = \vec{k}_{\text{min}}^2 - (E'_N - E_N)^2$. Another example is an inverse quadratic with two fit parameters, as suggested by Kelly [34] and used by Collins et al. [22]

$$G_E(Q^2) = \frac{G_E(0)}{1 + aQ^2 + \beta Q^4}, \quad (16)$$

with the charge radius obtained through $\langle r^2 \rangle_E = 6 \alpha$. Once the infinite-volume charge radii have been obtained, one then has best estimates for charge radii at any given set of lattice parameters.

As a demonstration of the method, lattice QCD results from QCDSF Collaboration [22] for the isovector nucleon electric charge radius are corrected to infinite volume, and shown in Fig. 6. The lattice calculation uses the two-flavor $O(a)$-improved Wilson quark action. The points displayed satisfy $m_{\pi}L > 3$, and the box sizes for each point range from 1.7 to 2.9 fm. The infinite volume form factors are calculated via

$$G_E(Q^2) = G'^{L}_E(Q^2) - (\delta_L[T(q^2)] - \delta_L[T(0)]), \quad (17)$$

with $T(q^2) = T_N(q^2) + T_{\Delta}(q^2) + T_{\text{tad}}(q^2)$. \quad (18)

In the construction of the charge radii, the $Q^2$-extrapolation Ansatz of Eq. (16) is used, to be consistent with Ref. [22]. Fig. 6 clearly shows that the infinite-volume points are larger in radius than the finite-volume points, and closer to the experimental value of $\langle r^2 \rangle_{E}^{\text{isov}} = 0.88 \text{ fm}^2$ [35,36].

The technique as described thus provides charge radii at different quark/pion masses, and hence enables the use of continuum $\chi$EFT to fit the quark mass dependence. Details of such an extrapolation will appear in a forthcoming paper.

4. Conclusion

Direct finite-volume corrections to charge radii are not well-defined on the lattice. The use of continuous derivatives in constructing the electric charge radius leads to inconsistent results in the finite-volume corrections. Alternatively, a satisfactory definition of radii can be achieved by implementing finite-volume corrections to the electric form factors directly, evaluated at discrete values of $q^2$. Subsequently, the resultant finite-volume-corrected form factors may then be converted into charge radii using an appropriate extrapolation in $Q^2$. A suitable definition of charge radius for comparison with experiment and continuum $\chi$EFT analysis has thus been obtained.

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Figure 6: (color online). Lattice QCD results for the isovector nucleon electric charge radius from QCDSF Collaboration at their original box sizes, and corrected to infinite volume.

References

[1] J. Gasser and H. Leutwyler, Nucl.Phys. B307, 763 (1988).

[2] D. B. Leinweber, A. W. Thomas, and R. D. Young, Phys.Rev.Lett. 92, 242002 (2004), hep-lat/0302020.

[3] R. D. Young, D. B. Leinweber, and A. W. Thomas, Phys.Rev. D71, 014001 (2005), hep-lat/0406001.

[4] D. B. Leinweber, S. Boinepalli, I. Cloet, A. W. Thomas, A. G. Williams, et al., Phys.Rev.Lett. 94, 212001 (2005), hep-lat/0406002.

[5] S. R. Beane, Phys. Rev. D70, 034507 (2004), hep-lat/0403015.

[6] J. Hall, D. Leinweber, and R. Young, Phys.Rev. D85, 094502 (2012), 1201.6114.

[7] R. D. Young, D. B. Leinweber, A. W. Thomas, and S. V. Wright, Phys.Rev. D66, 094507 (2002), hep-lat/0205017.
[8] D. B. Leinweber, S. Boinepalli, A. W. Thomas, P. Wang, A. G. Williams, et al., Phys.Rev.Lett. 97, 022001 (2006), hep-lat/0601025.

[9] B. C. Tiburzi, Phys.Rev. D77, 014510 (2008), 0710.3577.

[10] S. Syritsyn, J. Bratt, M. Lin, H. Meyer, J. Negele, et al., Phys.Rev. D81, 034507 (2010), 0907.4194.

[11] J. Bratt et al. (LHPC Collaboration), Phys.Rev. D82, 094502 (2010), 1001.3620.

[12] L. Greil, T. R. Hemmert, and A. Schafer, Eur.Phys.J. A48, 53 (2012), 1112.2539.

[13] J. M. M. Hall, D. B. Leinweber, and R. D. Young, Phys. Rev. D82, 034010 (2010), 1002.4924.

[14] D. B. Leinweber, R. Woloshyn, and T. Draper, Phys.Rev. D43, 1659 (1991).

[15] S. Nozawa and D. B. Leinweber, Phys. Rev. D42, 3567 (1990).

[16] D. B. Leinweber, T. Draper, and R. M. Woloshyn, Phys. Rev. D46, 3067 (1992), hep-lat/9208025.

[17] S. Boinepalli, D. Leinweber, A. Williams, J. Zanotti, and J. Zhang, Phys.Rev. D74, 093005 (2006), hep-lat/0604022.

[18] J. N. Hedditch et al., Phys. Rev. D75, 094504 (2007), hep-lat/0703014.

[19] S. Boinepalli et al., Phys. Rev. D80, 054505 (2009), 0902.4046.

[20] T. Yamazaki, Y. Aoki, T. Blum, H.-W. Lin, S. Ohta, et al., Phys.Rev. D79, 114505 (2009), 0904.2039.

[21] C. Alexandrou, M. Brinet, J. Carbonell, M. Constantinou, P. Harraud, et al., Phys.Rev. D83, 094502 (2011), 1102.2208.

[22] S. Collins, M. Gockeler, P. Hagler, R. Horsley, Y. Nakamura, et al., Phys.Rev. D84, 074507 (2011), 1106.3580.

[23] W. Detmold and M. J. Savage, Phys.Lett. B599, 32 (2004), hep-lat/0407008.
[24] S. R. Beane and M. J. Savage, Phys.Rev. D70, 074029 (2004),  
hep-ph/0404131.

[25] R. Young and A. Thomas, Phys.Rev. D81, 014503 (2010), 0901.3310.

[26] J. Hall, F. Lee, D. Leinweber, K. Liu, N. Mathur, et al., Phys.Rev. D84, 114011 (2011), 1101.4411.

[27] J. Hu, F.-J. Jiang, and B. C. Tiburzi, Phys.Lett. B653, 350 (2007), 0706.3408.

[28] F.-J. Jiang and B. Tiburzi, Phys.Rev. D78, 114505 (2008), 0810.1495.

[29] E. E. Jenkins and A. V. Manohar, Phys. Lett. B255, 558 (1991).

[30] E. E. Jenkins, Nucl. Phys. B368, 190 (1992).

[31] P. Wang, D. Leinweber, A. Thomas, and R. Young, Phys.Rev. D79, 094001 (2009), 0810.1021.

[32] R. F. Lebed, Phys. Rev. D51, 5039 (1995), hep-ph/9411204.

[33] T. Bauer, J. Bernauer, and S. Scherer (2012), 1209.3872.

[34] J. Kelly, Phys.Rev. C70, 068202 (2004).

[35] P. J. Mohr, B. N. Taylor, and D. B. Newell, Rev.Mod.Phys. 80, 633 (2008), 0801.0028.

[36] K. Nakamura et al. (Particle Data Group), J.Phys.G G37, 075021 (2010).