

Charmonium properties from lattice QCD + QED: Hyperfine splitting, J/ψ leptonic width, charm quark mass, and a_μ^c

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We have performed the first $n_f = 2 + 1 + 1$ lattice QCD computations of the properties (masses and decay constants) of ground-state charmonium mesons. Our calculation uses the Highly Improved Staggered Quark (HISQ) action to generate quark-line connected two-point correlation functions on MILC gluon field configurations that include u/d quark masses going down to the physical point, tuning the c -quark mass from $M_{J/\psi}$ and including the effect of the c quark's electric charge through quenched QED. We obtain $M_{J/\psi} - M_{\eta_c}$ (connected) = 120.3(1.1) MeV and interpret the difference with experiment as the impact on M_{η_c} of the η_c decay to gluons, missing from the lattice calculation. This allows us to determine $\Delta M_{\eta_c}^{\text{annihil}} = +7.3(1.2)$ MeV, giving its value for the first time. Our result of $f_{J/\psi} = 0.4104(17)$ GeV gives $\Gamma(J/\psi \rightarrow e^+e^-) = 5.637(49)$ keV, in agreement with, but now more accurate than, experiment. At the same time we have improved the determination of the c -quark mass, including the impact of quenched QED to give $\bar{m}_c(3 \text{ GeV}) = 0.9841(51)$ GeV. We have also used the time moments of the vector charmonium current-current correlators to improve the lattice QCD result for the c quark hadronic vacuum polarization (HVP) contribution to the anomalous magnetic moment of the muon. We obtain $a_\mu^c = 14.638(47) \times 10^{-10}$, which is 2.5σ higher than the value derived using moments extracted from some sets of experimental data on $R(e^+e^- \rightarrow \text{hadrons})$. This value for a_μ^c includes our determination of the effect of QED on this quantity, $\delta a_\mu^c = 0.0313(28) \times 10^{-10}$.

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I. INTRODUCTION

The precision of lattice QCD calculations has been steadily improving for some time and is now approaching, or has surpassed, the 1% level for multiple quantities. Good examples are the masses and decay constants of ground-state pseudoscalar mesons [1]. The meson masses can be used to tune, and therefore determine, quark masses. The decay constants can be combined with experimental annihilation rates to leptons to determine elements of the Cabibbo-Kobayashi-Maskawa matrix. The accuracy of

modern lattice QCD results means that sources of small systematic uncertainty that could appear at the percent level need to be understood. At this level QED effects, i.e., the fact that quarks carry electric as well as color charge, come into play. A naive argument that such effects could be $\mathcal{O}(\alpha_{\text{QED}})$ would imply a possible 1% contribution. One key driver for the lattice QCD effort to include QED effects has been that of calculations of the HVP contribution to the anomalous magnetic moment of the muon, a_μ . New results are expected soon from the Muon $g - 2$ experiment at Fermilab [2] which aims to clarify the observed tension between experiment and Standard Model theory seen by the Brookhaven E821 experiment [3]. Current lattice QCD calculations have reached the precision of a few percent for a_μ and the systematic uncertainties, for example from neglecting QED effects, have become a major focus of attention (see, for example, [4–6]).

QED effects can have large finite-volume corrections within a lattice QCD calculation because the Coulomb

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interaction is long range. For electrically neutral correlation functions, such as the ones needed for a calculation of the HVP, and that we study here, this is much less of an issue (and we demonstrate this). Since $\alpha_s^n \alpha_{\text{QED}}$ is not very different in size from α_{QED} at hadronic scales, calculations must be fully nonperturbative in QCD. A consistent calculation must also allow for the retuning of quark masses needed when QED effects are included.

Here we examine the properties of ground-state charmonium mesons more accurately than has been possible in previous lattice QCD calculations.¹ Since it is possible to obtain statistically very precise results for the charmonium system it is a good place to study small systematic effects from QED and other sources. We are able to see such effects in our results and quantify them. We include u , d , s and c quarks in the sea for the first time and have results on gluon field configurations with physical u/d sea quarks. We also analyze the impact of including an electric charge on the valence c quarks (only). This approximation, known as “quenched QED,” should capture the largest QED effects and enable us to see how much of a difference QED makes. For the vector (J/ψ) meson properties we improve on earlier results by using an exact method to renormalize the lattice vector current (both in QCD and QCD + QED). To tune the c -quark mass we use the J/ψ meson mass, taking into account the retuning that is required when QED is switched on. We find the impact of this to be of similar size to the more direct QED effects.

The quantities that we focus on here are the masses and decay constants of the ground-state η_c and J/ψ mesons, the c -quark mass and the contribution of the c vacuum polarization to a_μ .

The correlation functions that we calculate in our lattice QCD and QCD + QED calculations are “connected” correlation functions i.e., they are constructed from combining charm quark propagators from the source to the sink. We do not include diagrams in which the c and \bar{c} quarks annihilate to multiple gluons and hence hadrons. We can gain some insight into the effect this annihilation channel has on the meson masses by looking at the meson widths, which are twice the imaginary part of the mass and are dominated by hadronic channels. The J/ψ has a tiny width of 93 keV [1] but the pseudoscalar η_c can annihilate to two gluons, allowing it to mix with other flavor-singlet pseudoscalars, and it has a width of 32 MeV [1]. The annihilation channel might then be expected to have a larger impact on the η_c mass and lead lattice QCD calculations of the mass from connected correlators to disagree with experiment. The only way to achieve the $\mathcal{O}(1 \text{ MeV})$ accuracy required to see this is to determine the mass difference between the J/ψ and η_c (the hyperfine splitting). Any shift in the η_c

mass will have a much larger (by a factor of 30) relative effect in this splitting. Previous lattice QCD calculations of the hyperfine splitting from connected correlation functions have not been accurate enough to see a significant difference with experiment. Here, for the first time, we can see such a difference because we have very good control both of discretization effects and sea-quark mass effects and can also determine the impact of QED on this quantity.

A further place in which QED effects need to be quantified, given our accuracy, is that of the determination of the c -quark mass. We do this by tuning our results to the experimental J/ψ meson mass with and without electric charge on the valence c quarks and also determine the small change in the mass renormalization factor, Z_m , needed to convert to the standard $\overline{\text{MS}}$ mass.

Our analysis of the vector charmonium correlation functions with a completely nonperturbative renormalization of the vector current allows much improved accuracy in the determination of the leptonic decay width of the J/ψ . Using the same correlators, we determine the charm quark portion of the hadronic vacuum polarization contribution to the anomalous magnetic of the muon, $a_\mu^{\text{HVP},c}$, along with the impact of quenched QED on this quantity. We can compare this to phenomenological results from $R(e^+e^- \rightarrow \text{hadrons})$.

The paper is laid out as follows:

- (i) Section II describes the lattice QCD calculation and the inclusion of quenched QED;
- (ii) Section III describes our determination of the hyperfine splitting;
- (iii) Section IV, the c -quark mass;
- (iv) Section V, the J/ψ and η_c decay constants;
- (v) Section VI the time moments of c vector-vector correlators and the c -quark hadronic vacuum polarization contribution to a_μ ;
- (vi) Section VII gives our conclusions.

Each section of results includes a description of the pure QCD calculation followed by a determination of the impact of quenched QED on the result and then a discussion subsection including comparison to both experiment and previous lattice QCD calculations, where applicable. Finally Sec. VII collects up all of our results and summarizes our conclusions.

II. LATTICE SETUP

We perform calculations on a total of 17 gluon field ensembles, concentrating our analysis on 15 of these. Sixteen sets include the effects of light, strange and charm quarks in the sea with up and down quarks having the same mass ($n_f = 2 + 1 + 1$), one set has up and down quarks set separately to their physical values ($n_f = 1 + 1 + 1 + 1$). All gluon field ensembles include sea quarks using the HISQ action [8] and were generated by the MILC Collaboration [9,10]. Parameters for the ensembles are given in Table I. Our sets include lattices at 6 different β

¹For a different kind of lattice QCD calculation that maps out the spectrum more completely, but pays less attention to ground states, see [7].

TABLE I. Details of the lattice gluon field ensembles and calculation parameters used. The lattice spacing is determined from the Wilson flow parameter, w_0 [13], with w_0/a values given in column 2. The lattice spacing can be determined in fm by using $w_0 = 0.1715(9)$ fm [14] (fixed from f_π). L_s and L_t are the lattice spatial and temporal extents in lattice units. Columns 6, 7 and 8 give the sea quark masses in lattice units. Note that all of the configuration sets are $n_f = 2 + 1 + 1$, i.e., with equal mass u and d quarks (denoted l) *except* for set 3B which is $n_f = 1 + 1 + 1 + 1$. For set 3B am_u^{sea} and m_d^{sea} are listed separately with am_u^{sea} on top. am_c^{val} is the valence c -quark mass with ϵ_{Naik} the corresponding Naik parameter (see text). The column headed $N_{\text{cfg}} \times N_t$ shows both the number of configurations used in the pure QCD calculation and the number of time sources for propagators per configurations. $N_{\text{cfg,QED}}$ refers to the number of configurations (and time sources) used in QCD + QED calculations. Sets 1–3 will be referred to as very coarse ($a \approx 0.15$ fm), sets 4–8 as coarse ($a \approx 0.12$ fm), sets 9–11 as fine ($a \approx 0.09$ fm), 12 and 13 as superfine ($a \approx 0.06$ fm), 14 as ultrafine ($a \approx 0.045$ fm) and 15 as exafine ($a \approx 0.03$ fm).

| Set | β | w_0/a | L_s | L_t | am_l^{sea} | am_s^{sea} | am_c^{sea} | am_c^{val} | ϵ_{Naik} | $N_{\text{cfg}} \times N_t$ | $N_{\text{cfg,QED}} \times N_t$ |
|-----|---------|-------------|-------|-------|----------------------|---------------------|---------------------|---------------------|--------------------------|-----------------------------|---------------------------------|
| 1 | 5.80 | 1.1119(10) | 16 | 48 | 0.013 | 0.065 | 0.838 | 0.888 | -0.3820 | 1020 × 8 | ... |
| 2 | 5.80 | 1.1272(7) | 24 | 48 | 0.0064 | 0.064 | 0.828 | 0.873 | -0.3730 | 1000 × 8 | 340 × 16 |
| 3 | 5.80 | 1.1367(5) | 32 | 48 | 0.00235 | 0.0647 | 0.831 | 0.863 | -0.3670 | 1000 × 8 | ... |
| 3A | 5.80 | 1.13215(35) | 32 | 48 | 0.002426 | 0.0673 | 0.8447 | 0.863 | -0.3670 | 1762 × 16 | ... |
| 3B | 5.80 | 1.13259(38) | 32 | 48 | 0.001524 0.003328 | 0.0673 | 0.8447 | 0.863 | -0.3670 | 1035 × 16 | ... |
| 4 | 6.00 | 1.3826(11) | 24 | 64 | 0.0102 | 0.0509 | 0.635 | 0.664 | -0.2460 | 1053 × 8 | ... |
| 5 | 6.00 | 1.4029(9) | 24 | 64 | 0.00507 | 0.0507 | 0.628 | 0.650 | -0.2378 | ... | 340 × 16 |
| 6 | 6.00 | 1.4029(9) | 32 | 64 | 0.00507 | 0.0507 | 0.628 | 0.650 | -0.2378 | 1000 × 8 | 220 × 16 |
| 7 | 6.00 | 1.4029(9) | 40 | 64 | 0.00507 | 0.0507 | 0.628 | 0.650 | -0.2378 | ... | 220 × 16 |
| 8 | 6.00 | 1.4149(6) | 48 | 64 | 0.00184 | 0.0507 | 0.628 | 0.643 | -0.2336 | 1000 × 8 | ... |
| 9 | 6.30 | 1.9006(20) | 32 | 96 | 0.0074 | 0.037 | 0.440 | 0.450 | -0.1250 | 300 × 8 | ... |
| 10 | 6.30 | 1.9330(20) | 48 | 96 | 0.00363 | 0.0363 | 0.430 | 0.439 | -0.1197 | 300 × 8 | 371 × 16 |
| 11 | 6.30 | 1.9518(7) | 64 | 96 | 0.00120 | 0.0363 | 0.432 | 0.433 | -0.1167 | 565 × 8 | ... |
| 12 | 6.72 | 2.8941(48) | 48 | 144 | 0.00480 | 0.0240 | 0.286 | 0.274 | -0.0491 | 1019 × 8 | 265 × 16 |
| 13 | 6.72 | 3.0170(23) | 96 | 192 | 0.0008 | 0.022 | 0.260 | 0.260 | -0.0443 | 100 × 8 | ... |
| 14 | 7.00 | 3.892(12) | 64 | 192 | 0.00316 | 0.0158 | 0.188 | 0.194 | -0.0250 | 200 × 8 | ... |
| 15 | 7.28 | 5.243(16) | 96 | 288 | 0.00223 | 0.01115 | 0.1316 | 0.138 | -0.0127 | 100 × 4 | ... |

(the bare QCD coupling) values corresponding to 6 different sets of lattice spacing values with the finest lattice reaching a spacing of ~ 0.03 fm. Although “topology freezing” has been seen on the very finest lattices used here, we do not expect this to have significant impact on the charmonium quantities we study here because no valence light quarks are involved in the calculations [11]. We use ensembles with sea $u/d = l$ masses at the physical point on all but the finest two lattice spacings. We also employ three ensembles (sets 5, 6 and 7) with shared parameters except for their spatial extent in units of the lattice spacing L_s . These ensembles allow us to investigate finite-volume effects in our QED analysis. We test the impact of strong-isospin breaking effects in the sea by using two ensembles (sets 3A and 3B) with all parameters the same except that one ensemble has $m_u = m_d = m_l$ and one has $(m_u + m_d)/2 = m_l$ and $m_d/m_u = 2.18$. The gluon action on these ensembles is improved so that discretization errors through $\mathcal{O}(\alpha_s a^2)$ are removed [12].

On these gluon field configurations we calculate propagators for valence c quarks by solving the Dirac equation for a source consisting of a set of Gaussian random numbers across a time slice (a random wall source). We

use multiple time sources per configuration to improve statistical accuracy. The number of configurations used and the number of time sources is given in Table I. The table also gives the valence c -quark masses in lattice units, which may differ from those in the sea because they are tuned more accurately. This will be discussed further below. The HISQ action [8] includes an improved discretization of the covariant derivative in the Dirac equation. This removes tree-level a^2 discretization errors by the addition of a 3-link “Naik” term to the symmetric 1-link difference. For heavy quarks the coefficient of the Naik term is adjusted from 1 to $1 + \epsilon_{\text{Naik}}$ to remove $(am)^4$ errors at tree level [8]. A closed-form expression for ϵ in terms of the tree-level quark pole mass is given in [15] along with the formula for the tree-level quark pole mass in terms of the bare mass. Table I gives the values of ϵ that we use.

We combine charm quark and antiquark propagators to calculate two types of quark-line connected two-point correlation functions: pseudoscalar and vector. The ground state of the pseudoscalar correlation function corresponds to the η_c meson and the vector correlation function, to the J/ψ . When using staggered quarks, as here, the different spin structures are implemented using position dependent

phases in the operators at source and sink. The two-point ‘‘Goldstone’’ pseudoscalar ($\gamma_5 \otimes \gamma_5$ in spin-taste notation) correlation functions are simply constructed from quark propagators $S(x, 0)$ from the origin to x as

$$C(t) = \frac{1}{4} \sum_x \langle \text{Tr}(S(x, 0)S^\dagger(x, 0)) \rangle, \quad (1)$$

where the factor of 4 accounts for the taste multiplicity with staggered quarks. For the vector correlation functions we use a local vector operator (spin-taste $\gamma_i \otimes \gamma_i$). The correlation functions then combine $S(x, 0)$ with a propagator made from patterning the source with a phase $(-1)^{x_i}$ and inserting $(-1)^{x_i}$ at the sink time slice as we tie the propagators together and sum over spatial sites. Our vector correlation functions average over all spatial polarizations, i , for improved statistical precision. Note that we do not calculate any quark-line disconnected correlation functions.

The HISQ local vector current is not conserved and requires renormalization. For this purpose we use the RI-SMOM momentum subtraction scheme implemented on the lattice as discussed in [16]. In [16] it was shown that, because of the Ward-Takahashi identity, these renormalization factors do not suffer any contamination by non-perturbative artifacts (condensates) and can therefore be safely used in calculations such as those presented here. The quenched QED correction to the RI-SMOM vector current renormalization was also given in [16] and shown to be tiny ($\sim 0.01\%$) for the HISQ action (as expected since the pure QCD Z_V values only differ from 1 at the 1% level and quenched QED provides a small correction to this difference from 1). Here we use the Z_V values from [16] at a scale μ of 2 GeV. We will also demonstrate (see Sec. V) that using $\mu = 3$ GeV gives the same result as it must for a Z_V that correctly matches the lattice to continuum physics.

Since we make use of an ensemble (set 14) with a finer lattice spacing than those studied in [16] we have directly calculated the value of Z_V on set 14 at $\mu = 2$ GeV in addition. We have, however, only used a small number of configurations (6) in that calculation due to the computational limitation of the stringent Landau gauge fixing required. We therefore double the statistical uncertainty for Z_V on that ensemble. This has very little impact on our final results as the Z_V uncertainty is small. See the Appendix for a discussion of our Z_V values, where we also derive a Z_V value for set 15.

In order to tune the mass of the valence charm quark we use bare charm mass values on each lattice that produce a J/ψ mass equal to the experimental value (both in pure QCD and in QCD + QED). We choose the J/ψ here rather than the η_c because the relatively large width of the η_c means that annihilation effects that we are not including could lead to small (order 0.1%) uncertainties in the mass. This is mentioned in Sec. I and will be discussed further in Sec. III. We measure our valence c mass mistunings as the

difference between our lattice J/ψ mass and the experimental average value of 3.0969 GeV (with negligible uncertainty) [1]. The two panels of Fig. 2, where the horizontal line is the experimental value, show that our mistunings are well below 0.5%. These mistunings are allowed for in our final fits.

A. Two-point correlator fits

We fit the two-point correlation functions described above as a function of the time separation, t , between source and sink. The aim is to extract the energies (masses) and amplitudes (giving decay constants) of the ground-state mesons in each channel. However it is important to allow for the systematic effect of excited states that are present in the correlation functions and can affect the ground-state values if they are not taken into account. We do this by fitting the correlators to sums of exponentials associated with each energy eigenvalue and using Bayesian priors to constrain the (ordered) excited states in the standard way [17]. The pseudoscalar correlators are fit to

$$C_P(t) = \sum_i A_i^P f(E_i^P, t),$$

$$f(E, t) = e^{-Et} + e^{-E(L-t)}. \quad (2)$$

The vector correlators require a more complicated form because of the presence of opposite parity states as a result of the use of staggered quarks:

$$C_V(t) = \sum_i (A_i^V f(E_i^V, t) - (-1)^t A_i^{V,o} f(E_i^{V,o}, t)). \quad (3)$$

We cut out the correlator values at low values of t , below some value t_{\min} (5–10) where excited state contamination is most pronounced. We also use a standard procedure (see Appendix D of [18]) to avoid underestimating the low eigenvalues of the correlation matrix and hence the uncertainty.

The fit parameters that we need from Eqs. (2) and (3) are the mass of the ground state (E_0^P and E_0^V) and the amplitude (A_0^P and A_0^V). From the amplitude we determine the decay constant, see Sec. V.

B. QED formalism

We perform calculations in both lattice QCD and in lattice QCD with quenched QED. By quenched QED we mean that we include effects from the valence quarks having electric charge but we neglect effects from the electric charge of the sea quarks. We will first describe how we include QED and then discuss the expected impact on our results of not including the QED effects from the sea quarks.

To include quenched QED effects we generate a random momentum space photon field $A_\mu(k)$ in Feynman gauge for each QCD gluon field configuration. This choice of gauge simplifies the generation of the photon field as the QED

path integral weight takes the form of a Gaussian with variance $1/\hat{k}^2$ where $\hat{k} = 2 \sin(k_\mu/2)$. The results presented here do not depend on this gauge choice. Once the momentum space field is generated zero modes are set to zero using the QED_L formulation [19]. A_μ is then Fourier transformed into position space. We have checked that these Feynman gauge A_μ fields produce the plaquette and average link expected from $\mathcal{O}(\alpha_{\text{QED}})$ perturbation theory (readily obtained from $\mathcal{O}(\alpha_s)$ calculations in lattice QCD with Wilson glue [20,21]). These gauge fields are exponentiated as $\exp(i e Q A_\mu)$ to give a U(1) field which is then multiplied into the QCD gauge links before HISQ smearing. Q is the quark electric charge in units of the proton charge e .

This approach is known as the stochastic approach to quenched QED [22], in contrast to the perturbative approach of [23]. Since $\mathcal{O}(\alpha_{\text{QED}})$ is already a very small effect, we are seeking here only to pin down the linear term in α_{QED} , fully nonperturbatively in α_s . The two approaches should then give the same result to our level of accuracy; we use the stochastic approach because it is more straightforward (in the quenched case) and gives very precise results for the c quarks we are interested in here.

C. Impact of quenching QED

Quenched QED affects only the valence quarks; the sea quarks remain uncharged. We expect the valence quark contribution to be by far the largest QED effect (although already very small as we will see) and discuss here the small systematic error that remains from ignoring sea-quark QED effects. The impact of having $m_u = m_d$ in the sea for most of our results is at the same level and we also discuss that.

We first discuss the determination of the lattice spacing in QCD with quenched QED. In such a calculation there is no coupling of QED effects to purely gluonic quantities. This means that the Wilson flow parameter w_0/a , measured on each ensemble, is unchanged from pure QCD. The physical value of w_0 that is used to determine the lattice spacing on each ensemble was determined in [14] by matching the decay constant of the π meson, f_π , in lattice QCD to that obtained from experiment. The experimental value of f_π is obtained from measurement of the rate for $\pi \rightarrow \ell \nu[\gamma]$ decay where $[\gamma]$ indicates that the rate is fully inclusive of additional photons. The rate obtained is then adjusted to remove electromagnetic and electroweak corrections and to give a “purely leptonic rate” corresponding to weak annihilation at lowest order in the absence of QED [1]. Combining this with a determination of $|V_{ud}|$ from nuclear β decay [1] gives an experimental value of $f_\pi \equiv f_\pi^{\text{expt}}$ which is a “pure QCD” value, albeit that for a physical π^+ meson. The dominant uncertainty in f_π^{expt} is that from the remaining uncertainty in the electromagnetic corrections to the experimental rate, mainly from the hadronic-structure dependent contributions to the emission of additional photons. This is set at 0.1% in [1].

Because f_π^{expt} is a pure QCD quantity it can be used to set the lattice spacing in lattice QCD in a way that should be minimally different for lattice QCD + QED.² Small differences might still be expected between the lattice QCD f_π and the experimental value from the way that the quark masses are tuned in a pure QCD scenario. The lattice QCD calculation in [14] used $m_u = m_d$ and tuned the average mass, m_l , to the experimental mass of the π^0 , which is the mass that both neutral and charged π mesons have in the absence of QED, up to quadratic corrections in the $u - d$ mass difference. An uncertainty was included in the π^0 mass to allow for these corrections, taking an estimate from chiral perturbation theory [25]. We expect the impact of such effects to be tiny, well below 0.1%. They are at the same level as potential effects from QED in the sea and would therefore be only possible to pin down with a calculation that included the impact of having electrically charged quarks in the sea.

These expectations are backed up by recent lattice QCD + QED results [6] that used the Ω baryon mass to determine w_0 . The impact of QED for the sea quarks was included to first order in α_{QED} . No effects linear in $m_u - m_d$ are expected in M_Ω because, like f_π and M_π above, it is symmetric under $u \leftrightarrow d$ interchange. Strong-isospin breaking effects were therefore ignored. The impact of QED in the sea on $w_0 M_\Omega$ was found to be $\mathcal{O}(0.01\%)$, whereas the effect of QED for the valence quarks (already allowed for in the f_π analysis) was $\mathcal{O}(0.05\%)$. The final value of w_0 using M_Ω from [6] agrees well with the result using f_π from [14], although the uncertainties in both cases are completely dominated by those from the pure QCD, isospin-symmetric part of the calculation.

From this we conclude that, at the sub-0.1% level, we can compare lattice QCD plus quenched QED with pure lattice QCD using the same value of the lattice spacing, determined from f_π , in both calculations.

The impact of quenching QED on charmonium quantities follows a similar discussion to that for the lattice spacing because interaction with the electric charge of the sea quarks is suppressed by sea quark mass effects and by powers of α_s . Since the sum of electric charges of u , d and s sea quarks is zero, QED interaction between valence c quarks and light sea quarks will be suppressed by sea-quark mass differences. The impact of c quarks in the sea is already small and so we can safely neglect the even smaller QED effects from valence/sea c quark interactions. The leading sea-quark QED effect will then come from photon exchange across a sea-quark bubble at $\mathcal{O}(\alpha_s^2 \alpha_{\text{QED}})$ [16] in perturbative language. The expected size is then 10% of that of the QED effects from valence c quark interactions,

²Indeed, f_π cannot readily be calculated in lattice QCD + QED because of infrared QED effects from an electrically charged π^+ . Calculations have been done that confirm the size of radiative corrections to f_π , however [24].

which we will see are themselves typically a small fraction of 1%.

D. Impact of having $m_u = m_d$ in the sea

As discussed above, we expect the effects of having $m_u = m_d$ in the sea, i.e., not including strong-isospin breaking effects, to be negligible. For both the scale-setting determination and for the charmonium quantities themselves, pure strong-isospin breaking effects are quadratic in $(m_u - m_d)/\Lambda$. Effects linear in the sea-quark masses are already small, for example an $\mathcal{O}(5 \text{ MeV})$ shift in the average u/d quark mass produces a 1% effect on w_0/a [26]. We might then expect quadratic effects to be $\mathcal{O}(0.01\%)$.

We can provide a test of these expectations from results on gluon ensemble sets 3A and 3B that differ only in the values of m_u and m_d in the sea for the same average (which has its physical value). Set 3B has m_d/m_u set to the expected ratio [27]. We see from Table I that the determinations of w_0/a agree at the level of their 0.03% uncertainties. In contrast, the w_0/a value on set 3A differs by a clearly visible 0.40(5)% from that on set 3, which has sea-quark masses that are slightly mistuned from the physical point by an amount (summing over u , d and s) equal to 5% [26] of m_s .

Table II compares values for the J/ψ and η_c masses in lattice units on these two ensembles for the same am_c^{val} and the ratio of the two results is plotted in Fig. 1. The meson masses in lattice units agree on the two ensembles to within their statistical errors which are at the level of 0.001%. We also tabulate results for the decay constants and plot the ratio of these values. Again agreement is seen between results on set 3A and set 3B. They provide a weaker constraint because of much larger statistical errors, but nevertheless they agree within 0.05%. Notice that this comparison does not allow for possible changes in w_0/a in the two cases. As discussed above, this could be at the 0.01% level. Again we can contrast the agreement between sets 3A and 3B with the results on set 3 where, for the same am_c^{val} , the η_c mass differs by 0.02%.

TABLE II. Results for the η_c and J/ψ masses and decay constants (see Sec. V for how these are calculated) in lattice units on gluon field ensembles sets 3A and 3B (Table I). Both sets have the average u/d quark mass in the sea set to its physical value but set 3B has m_d/m_u also set to the expected ratio. The valence c -quark mass was set to 0.863 in lattice units.

| | 3A ($n_f = 2 + 1 + 1$) | 3B ($n_f = 1 + 1 + 1 + 1$) |
|-------------------|--------------------------|------------------------------|
| aM_{η_c} | 2.288139(19) | 2.288131(25) |
| $aM_{J/\psi}$ | 2.375618(44) | 2.375585(60) |
| af_{η_c} | 0.366596(38) | 0.366588(41) |
| $af_{J/\psi}/Z_V$ | 0.41799(16) | 0.41790(24) |

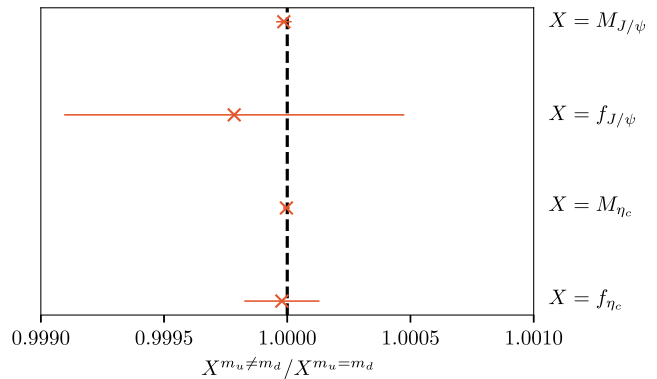


FIG. 1. A test of the impact of strong-isospin breaking in the sea through a comparison of results for the charmonium quantities given in Table II for sets 3A and 3B (Table I). These sets differ only in the u/d quark masses in the sea. Set 3A has $m_u = m_d$ and set 3B has $m_d/m_u = 2.18$ with the same average value. The plot above gives the ratio of results in lattice units, for the same am_c^{val} , for the J/ψ and η_c masses and decay constants. The masses agree to within their 0.001% statistical errors and the decay constants agree to within their statistical errors (0.05% for the J/ψ).

We conclude that we can safely neglect strong-isospin breaking in the sea and proceed with calculations on gluon field ensembles with $m_u^{\text{sea}} = m_d^{\text{sea}}$.

E. A first look at quenched QED effects

An estimate of the size of corrections from quenched QED (often simply referred to as QED in what follows) in charmonium systems can be obtained by studying the effect on the J/ψ mass. The bottom panel of Fig. 2 shows the J/ψ mass for the same valence c mass for both QCD + QED and pure QCD calculations on sets 2, 6, 10 and 12. The QCD + QED and QCD results at the same lattice spacing are separated on the x axis for clarity. All points share a correlated uncertainty (the outer error bar) from w_0 and this dominates the uncertainty. The uncorrelated error is shown by the smaller inner error bar. Note that the points at the same lattice spacing are also correlated through their w_0/a value. The shift of the mass in QCD + QED compared to pure QCD is very small, at the level of 0.1%, and is upwards.

When discussing QCD + QED and pure QCD calculations of some quantity X we will use the notations $X[\text{QCD} + \text{QED}]$ and $X[\text{QCD}]$ respectively. We will often consider the ratio of the two for which we will use the shortened notation $R_{\text{QED}}^{(0)}[X]$. R_{QED}^0 will refer to the “bare” ratio defined using the same bare quark mass am_c in both QCD + QED and pure QCD calculations. R_{QED} will refer to the final QED-renormalized ratio which includes the impact of retuning the c -quark mass to give the experimental J/ψ mass in both the QCD + QED and pure QCD cases. So

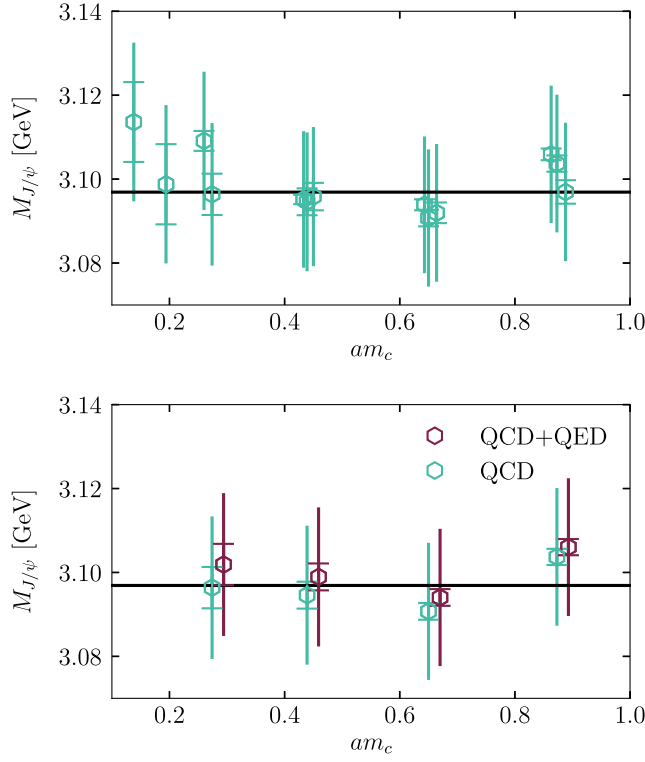


FIG. 2. Top panel: Pure QCD J/ψ masses on all 15 sets from Table I using the valence masses in that table. Two error bars are shown. The error can be broken into parts that are uncorrelated between different sets and the contribution from fixing the lattice spacing from the physical value of w_0 which is correlated. The outer error bar shows the full uncertainty and the inner bar the uncertainty without the contribution from w_0 . Bottom panel: The J/ψ masses on sets 2, 6, 10 and 12 with and without the inclusion of quenched QED. On each set the same valence mass (and lattice spacing) was used for both pure QCD and QCD + QED but the points have been separated on the x axis for clarity. The error bars are the same as for the top panel, but note that here there is a correlation of the uncertainty from w_0/a for the QCD and QCD + QED results on each set. The QCD + QED results are above the pure QCD results in every case.

$$R_{\text{QED}}^0[X] \equiv \frac{X[\text{QCD} + \text{QED}]}{X[\text{QCD}]} \Big|_{\text{fixed } am_c}$$

$$R_{\text{QED}}[X] \equiv \frac{X[\text{QCD} + \text{QED}]}{X[\text{QCD}]} \Big|_{\text{fixed } M_{J/\psi}}. \quad (4)$$

As shown in Fig. 2 the bare c -quark mass has to be readjusted downwards for QCD + QED relative to pure QCD.

F. Fitting strategy

We have results in pure QCD for all of the sets in Table I and QCD + QED results on a subset of ensembles. To be able to simultaneously account both for the “direct” effects of QED and for the effects of valence c mass mistuning,

which may be similarly sized, we choose to fit all of this data in a single fit for each quantity we consider. The generic form of the fit we use for a quantity X is

$$X(a^2, Q)$$

$$= x \left[1 + \sum_{i=1}^5 c_a^{(i)} (am_c)^{2i} \right.$$

$$+ c_{m,\text{sea}} \delta_m^{\text{sea},uds} \{ 1 + c_{a^2,\text{sea}} (\Lambda a)^2 + c_{a^4,\text{sea}} (\Lambda a)^4 \}$$

$$+ c_{c,\text{sea}} \delta_m^{\text{sea},c} + c_{c,\text{val}} \delta_m^{\text{val},c}$$

$$\left. + \alpha_{\text{QED}} Q^2 \left\{ c_{\text{QED}} + \sum_{p=1}^3 c_{aQ}^{(p)} (am_c)^{2p} + c_{\text{val},Q} \delta_m^{\text{val},c} \right\} \right]. \quad (5)$$

Here Q is the valence quark electric charge (in units of e) used in the calculation and is therefore 0 in pure QCD. The pure QCD value of this fit at the physical point (the continuum limit with quark masses set to their physical values) is x . The value including quenched QED corrections is $x[1 + \alpha_{\text{QED}} Q^2 c_{\text{QED}}]$. Note that the factor of α_{QED} multiplying the QED part of the fit function is there so that the fit parameters are order 1. The stochastic method that we use includes in principle all orders of α_{QED} but we expect to see only linear terms, including $\alpha_{\text{QED}} \alpha_s^n$ pieces.

Our fits are typically to 15 pure QCD data points and 4 QCD + QED points. The pure QCD points do not include those on sets 6 and 7 which are used to test finite-volume effects or on sets 3A and 3B that are used to test strong-isospin breaking effects, but they do include additional results at mistuned c -quark masses to test mistuning effects.

We now describe each of the terms in Eq. (5) in turn. The $(am_c)^i$ terms on the first line account for discretization effects. Because we are dealing with heavy quarks here, the scale of discretization effects can be set by m_c and will typically be larger than those for light-quark quantities. Since $m_c > \Lambda_{\text{QCD}}$ any discretization effects set by scale Λ_{QCD} will simply appear as m_c -scale discretization effects with a small coefficient.

The terms on the second line allow for mistuning of the sea u/d and s masses and discretization effects in that mistuning (we shall see that those are important for the hyperfine splitting). The total of the mistuning of the sea masses is defined as in [26]:

$$\delta_m^{\text{sea},uds} = \frac{2m_l^{\text{sea}} + m_s^{\text{sea}} - 2m_l^{\text{phys}} - m_s^{\text{phys}}}{10m_s^{\text{phys}}}. \quad (6)$$

m_s^{phys} is taken from [26] or, where not available on the finest lattices, calculated from the tuned c -quark mass and the m_c/m_s ratio given in [26]. The value of Λ in the discretization effects multiplying the sea-quark mistuning is taken as 1 GeV ($\sim m_c$).

The effect of mistuning the charm mass in the sea is included in the third line of Eq. (5) using

$$\delta_m^{\text{sea},c} = \frac{m_c^{\text{sea}} - m_c^{\text{phys}}}{m_c^{\text{phys}}}. \quad (7)$$

The values of m_c^{phys} are taken from [26]. Although this used a slightly different tuning method the differences are negligible for this purpose. We have tested that including discretization effects for this term has no effect on the fit.

Mistuning in the valence mass is accounted for through $\delta_m^{\text{val},c}$ on the third and fourth lines of Eq. (5). We define this as

$$\delta_m^{\text{val},c} = \frac{M_{J/\psi} - M_{J/\psi}^{\text{expt}}}{M_{J/\psi}^{\text{expt}}}, \quad (8)$$

where $M_{J/\psi}$ is our lattice result for that ensemble in either the QCD or the QCD + QED case. Thus $\delta_m^{\text{val},c}$ is zero (the valence c -quark mass is tuned) when the J/ψ mass takes its experimental value on each ensemble (and with or without QED). The fit parameters $c_{c,\text{val}}$ and $c_{\text{val},Q}$ then determine the dependence on the valence c mass of the quantity being fit, and the QED corrections to that dependence, respectively. The experimental value of the J/ψ mass is 3.0969 GeV [1] with negligible uncertainty.

In order to make use of the correlations between our QCD + QED and pure QCD results on the same gluon field configurations we perform simultaneous fits to the correlators in each case. The fits then capture the correlations and we can propagate them to the fit of Eq. (5). At the same time it allows us to determine the ratio of QCD + QED to pure QCD for the quantities that we will study. We will give results for these ratios in the sections that follow.

The fit form of Eq. (5) has been constructed such that the coefficients (apart from x) are expected to be of order 1. We therefore use priors of 0 ± 1 for all fit parameters except x for which we take a prior width on its expected value of 20% (the prior mean for x depends on the quantity being fitted).

III. HYPERFINE SPLITTING

A. Pure QCD

The hyperfine splitting, ΔM_{hyp} , is calculated on each ensemble as the difference of the vector and pseudoscalar ground-state masses, in lattice units, divided by the lattice spacing. The results for aM_{η_c} and $aM_{J/\psi}$ and their difference are given in Table III for the pure QCD case. Although the pseudoscalar and vector correlators on each configuration are correlated the fit outputs for the vector correlator dominate the uncertainties and so the correlations have very little effect as a result.

The pure QCD results are plotted in Fig. 3 along with the fit form of Eq. (5) for the pure QCD case (i.e., $Q = 0$). Note

TABLE III. The η_c and J/ψ masses and their difference ($a\Delta M_{\text{hyp}}$) in pure QCD on each set in lattice units. The values of am_c^{val} are those given in Table I except for two cases with a deliberately mistuned c -quark mass: set 6 denoted by a * where $am_c = 0.643$ and set 14 denoted by a † where $am_c = 0.188$. The pseudoscalar and vector correlator fits have been performed separately and the correlations between aM_{η_c} and $aM_{J/\psi}$ have therefore been ignored because they have little impact.

| Set | aM_{η_c} | $aM_{J/\psi}$ | $a\Delta M_{\text{hyp}}$ |
|-----|---------------|---------------|--------------------------|
| 1 | 2.331899(72) | 2.42072(19) | 0.08883(20) |
| 2 | 2.305364(39) | 2.39308(14) | 0.08772(14) |
| 3 | 2.287707(26) | 2.37476(21) | 0.08705(21) |
| 4 | 1.876536(48) | 1.94364(10) | 0.06710(11) |
| 6 | 1.848041(35) | 1.914749(67) | 0.066708(76) |
| 6* | 1.834454(34) | 1.901479(66) | 0.067025(74) |
| 8 | 1.833950(18) | 1.900441(39) | 0.066491(43) |
| 9 | 1.366839(72) | 1.41568(16) | 0.04884(17) |
| 10 | 1.342455(21) | 1.391390(43) | 0.048935(48) |
| 11 | 1.329313(18) | 1.378237(51) | 0.048924(54) |
| 12 | 0.896675(24) | 0.929860(54) | 0.033185(59) |
| 13 | 0.862689(22) | 0.895650(37) | 0.032961(43) |
| 14 | 0.666818(39) | 0.691981(54) | 0.025163(67) |
| 14† | 0.652439(56) | 0.67798(14) | 0.02554(15) |
| 15 | 0.496991(47) | 0.516126(68) | 0.019135(82) |

the small range of the y axis—this is possible for our results because we have a highly improved quark action with small discretization errors. Since all tree-level a^2 errors have been removed, the shape of the curve reflects the fact that higher-order a^4 and a^6 errors are visible; discretization errors of this kind are present in all formalisms of course, but often they are hidden below much larger a^2 effects and consequently overlooked. Note also the clear dependence on the light sea-quark mass seen on the finest lattices. To pin down the value of the valence mass mistuning parameter, c_{val} , we include results at deliberately mistuned c -quark masses (see Table III). These are not shown in the figure but are included in the fit. The result for the hyperfine splitting in the pure QCD case in the continuum limit and for physical quark masses is 118.6(1.1) MeV, which is higher than the experimental average value, as is clear in Fig. 3. In order to understand what this means, we need to quantify all possible sources of small systematic effects in our calculation, including those from QED.

B. Impact of quenched QED

The fractional direct effect of quenched QED on the η_c and J/ψ masses and the hyperfine splitting are given in Table IV. The correlation between the QCD + QED and the pure QCD results enables very high statistical accuracy to be obtained in the ratio. The inclusion of quenched QED shifts both the η_c and J/ψ masses up by $\mathcal{O}(0.1\%)$,

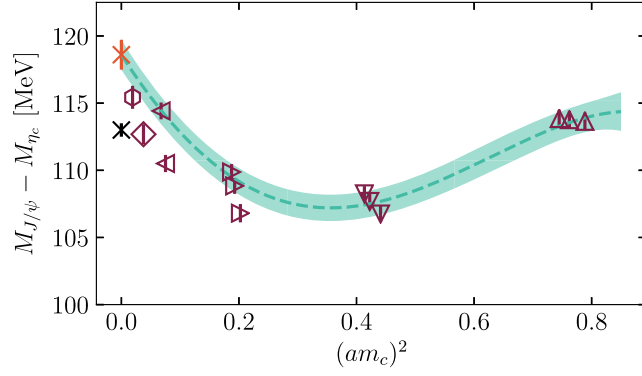


FIG. 3. The charmonium hyperfine splitting as a function of lattice spacing on pure QCD ensembles. Our results are from ensembles including u , d , s and c quarks in the sea with varying c -quark mass retuning effects. The raw lattice results, for well-tuned c -quark masses, are given by symbols with error bars. The error bars include both statistical uncertainties and those from determining the lattice spacing from w_0 , which are correlated between values. The results on each group of ensembles with approximately the same lattice spacing are given the same symbol. Within these groups, the results go from right to left as the u/d quark mass changes from $m_s/5$ to the physical value. Notice the small range on the y axis; this is the result of discretization effects being so small for the HISQ action. Results at mistuned c masses are not plotted but are included in the fit. The fit line is the output of the fit from Eq. (5) at physical quark masses and with $Q = 0$. The orange cross gives our result in the continuum limit for physical quark masses. The black cross gives the experimental average result [1].

depending on lattice spacing, at a given am_c value. Although these mass shifts are small, there is a difference between the shift for the J/ψ and that for η_c and so the inclusion of quenched QED also changes the hyperfine splitting. The impact here is more substantial, 0.7%, because the hyperfine splitting is so much smaller. The size of the direct QED effect on the hyperfine splitting can be simply estimated by replacing $C_F\alpha_s$ by $Q^2\alpha_{\text{QED}}$ in a potential model estimate of the splitting. This gives a fractional effect of $\alpha_{\text{QED}}/(3\alpha_s)$, consistent with what we find.

TABLE IV. QCD + QED η_c and J/ψ masses and hyperfine splitting presented as the ratio of the QCD + QED result to the pure QCD one on that set. Correlations between the calculations in the QCD + QED and pure QCD cases are used in the determination of the ratio and result in the very high statistical accuracy obtained. Note that the ratio is calculated for the same am_c value in the two cases i.e., the ratio given here does *not* include the impact of retuning the c -quark mass.

| Set | $R_{\text{QED}}^0[M_{\eta_c}]$ | $R_{\text{QED}}^0[M_{J/\psi}]$ | $R_{\text{QED}}^0[\Delta M_{\text{hyp}}]$ |
|-----|--------------------------------|--------------------------------|---|
| 2 | 1.000450(26) | 1.000750(27) | 1.0086(10) |
| 6 | 1.0008335(59) | 1.0010742(81) | 1.00774(28) |
| 10 | 1.0011861(54) | 1.0014044(76) | 1.00739(26) |
| 12 | 1.0015755(48) | 1.001787(11) | 1.00750(33) |

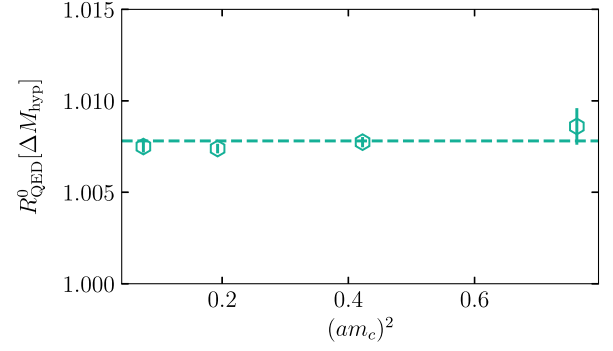


FIG. 4. The fractional effect of quenched QED on the charmonium hyperfine splitting plotted against $(am_c)^2$. The fractional effect is determined at the same am_c value, i.e., it does not include c -quark mass retuning effects. The dashed line is horizontal and shows the weighted average value. The results show the precision that can be obtained by capitalizing on the correlations between QCD + QED and QCD. This enables a clear demonstration that the impact of quenched QED here is not dependent on the lattice spacing.

The values of $R_{\text{QED}}^0[\Delta M_{\text{hyp}}]$ are plotted against $(am_c)^2$ in Fig. 4. This shows that the results are consistent across all lattice spacings and thus discretization effects in this ratio are smaller than for the masses themselves.

Finite-volume effects are an issue in general for QED corrections to meson masses but we expect them to be small for the electrically neutral and spatially small charmonium mesons that we study here. In [28] it is shown that the finite-volume expansion for electrically neutral mesons starts at $\mathcal{O}(1/L_s^4)$. In Fig. 5 we compare results for the fractional effect of QED on the J/ψ and η_c as a function of $1/L_s$. This calculation is done on sets 5, 6 and 7 (see Table I) which differ only in their spatial extent. We see no finite-volume effects to well within 0.01%, and we therefore ignore such effects.

Our results including both pure QCD and QCD + QED are shown in Fig. 6, plotted against $(am_c)^2$. The fit curve

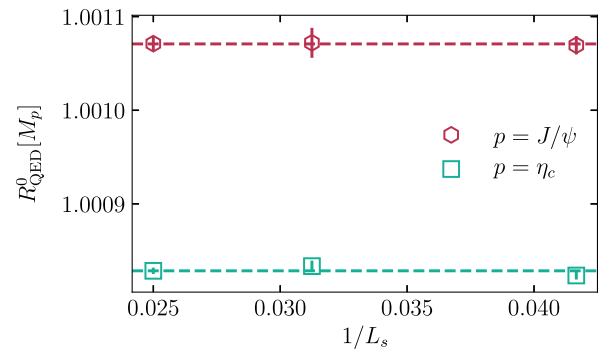


FIG. 5. The fractional shift in the J/ψ and η_c masses from the inclusion of quenched QED plotted as a function of $1/L_s$ on sets 5, 6 and 7. The dashed lines are horizontal lines at the weighted average values.

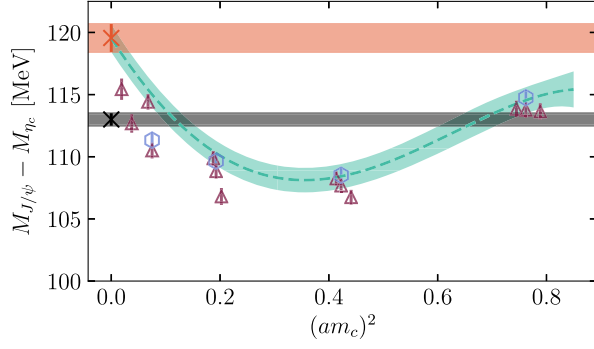


FIG. 6. The charmonium hyperfine splitting as a function of lattice spacing, including both QCD + QED and pure QCD points. The red open triangles are the same lattice results as in Fig. 3. The additional QCD + QED points are given as blue open hexagons. The green fit band is the output of the fit from Eq. (5), but now with the c quark electric charge, $Q = 2/3$. The orange cross and orange band gives our result in the continuum limit for physical quark masses. The black cross and black band gives the experimental average result [1].

from Eq. (5) at physical quark masses is also shown. The fit has a $\chi^2/\text{d.o.f.}$ of 0.59 and gives a hyperfine splitting in the continuum limit at physical quark masses of 119.6 (1.1) MeV. In Fig. 7 we show the results of a stability analysis for this fit. The figure shows that the fit is very robust.

Taking the (correlated) ratio between the physical value of the full QCD + QED fit and the physical value from the fit at $Q = 0$ (i.e., the pure QCD result) we obtain $R_{\text{QED}}[\Delta M_{\text{hyp}}] = 1.00804(43)$. This ratio now does include the effect of retuning the c -quark mass to obtain the experimental J/ψ mass when quenched QED is included. This retuning requires a reduction of the bare c quark mass by $\mathcal{O}(0.1\%)$ (see Table IV) and this further increases the

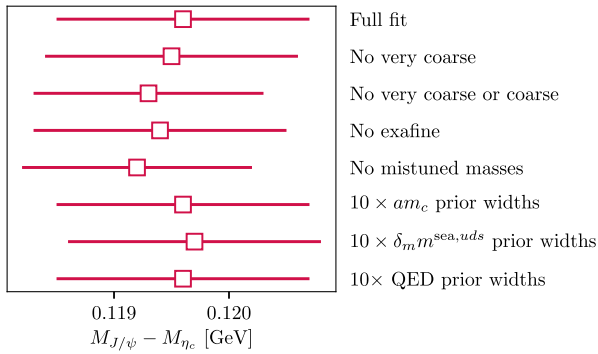


FIG. 7. A stability analysis for our fit (see text) to the charmonium hyperfine splitting. Our full fit result is shown at the top. The lines with error bars below this show the result for different modifications of this fit. From the top, these include missing out results on particular sets of configurations, then missing out the results using mistuned c -quark masses and then changing the priors by a factor of 10 on different sets of parameters in the fit.

hyperfine splitting, but only by $\mathcal{O}(0.1\%)$. The impact of QED here is therefore dominated by the direct quenched QED effect.

There is an additional pure QED contribution to the J/ψ mass that has not been included yet since it is quark-line disconnected. This comes from a diagram in which the $c\bar{c}$ annihilate into a photon which converts back into $c\bar{c}$. The contribution of this diagram is

$$\frac{8\pi\alpha_{\text{QED}}Q^2}{M_{J/\psi}^2} |\psi(0)|^2, \quad (9)$$

where $\psi(0)$ is the nonrelativistic J/ψ wave function equal (in the normalization being used here) to $f_{J/\psi} \sqrt{M_{J/\psi}} / \sqrt{6}$ [29]. The contribution evaluates to +0.7 MeV, which is a tiny, and completely negligible, effect for the J/ψ meson mass (0.03%). It has some impact on the hyperfine splitting because that is 30 times smaller and so we include it here. We add this contribution to our hyperfine splitting result with a 30% uncertainty from possible QCD corrections to give a final result of

$$M_{J/\psi} - M_{\eta_c}(\text{connected}) = 120.3(1.1) \text{ MeV}. \quad (10)$$

The error budget for our hyperfine splitting result is given in Table V. We follow Appendix A of [30] for the meaning of the uncertainties contributing to the error budget. The majority of the uncertainty is associated with the lattice spacing determination, either from the correlated w_0 uncertainty or the individual w_0/a uncertainties. This is not surprising because the hyperfine splitting is sensitive to uncertainties in the determination of the lattice spacing for the reasons discussed in [31]. We have separated out the uncertainty arising from the pure QCD data and the $R_{\text{QED}}^0[\Delta M_{\text{hyp}}]$ values from Table IV which we label “Pure QCD Statistics” and “QCD + QED Statistics” in Table V. The sea mistuning uncertainty comes from the c_m coefficients in Eq. (5) and the valence mistuning

TABLE V. Error budget for our final result for the charmonium hyperfine splitting including quenched QED corrections. The uncertainties shown are given as a percentage of the final result. The largest uncertainties are clearly from the determination of the lattice spacing.

| | ΔM_{hyp} |
|----------------------|-------------------------|
| $a^2 \rightarrow 0$ | 0.13 |
| Pure QCD statistics | 0.24 |
| QCD + QED statistics | 0.08 |
| w_0/a | 0.24 |
| w_0 | 0.87 |
| Valence mistuning | 0.02 |
| Sea mistuning | 0.06 |
| Total | 0.96 |

uncertainty from the c_{val} and $c_{\text{val},Q}$ coefficients. The $a^2 \rightarrow 0$ uncertainty is from the c_a and c_{aQ} coefficients.

Our final result is for the charmonium hyperfine splitting determined from quark-line connected correlation functions in QCD and including the impact of QED effects, through explicit calculation in quenched QED. We expect the effect of further QED effects in the sea to be negligible compared to our 1% uncertainty. The only significant Standard Model effect then missing is that of quark-line disconnected diagrams in which the $c\bar{c}$ annihilate to gluons. We expect this effect to be much larger for the η_c than for the J/ψ so a comparison of our result for the hyperfine splitting to experiment can yield information on the size and sign of the annihilation contribution to the η_c mass. This is discussed in the next subsection.

C. Discussion: Hyperfine splitting

The experimental average value of the hyperfine splitting [113.0(5) MeV] from the Particle Data Group (PDG) [1] is calculated as the difference of the separate averages for the J/ψ and η_c masses. The different experimental results contributing to the PDG average of the two masses are shown in Fig. 8. For the J/ψ mass the average is dominated

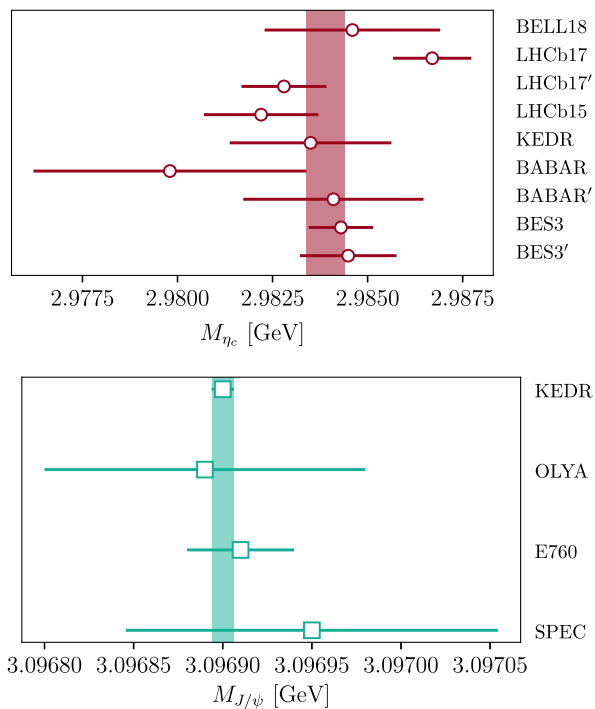


FIG. 8. Comparison of different experimental results for the J/ψ and η_c masses along with the PDG average values. The η_c results represent a recent subset of those used in the PDG average. The most recent result is from BELLE (denoted BELL18) [36]. There are three different determinations from LHCb [34,35,37], two of which also measured the hyperfine splitting. We include a KEDR measurement [33], two from different BABAR analyses [38] and two from BESIII [39,40].

by the most recent result from KEDR [32]. There are only three experimental results used in these analyses that can independently produce values for the hyperfine splitting. These are the KEDR experiment [32,33] and two LHCb analyses in different channels [34,35]. The LHCb result in [35] used the $\eta_c(2S) \rightarrow p\bar{p}$ decay while the analysis of [34] used $\eta_c(1S) \rightarrow p\bar{p}$. In the comparison plot of Fig. 9 [34] is referred to as LHCb15 and [35] as LHCb17.

Figure 9 shows a comparison of lattice QCD results for the charmonium hyperfine splitting along with the PDG average value and separate experimental values that measured this splitting. Previous calculations on gluon field configurations that included $n_f = 2 + 1$ flavors of sea quarks by HPQCD [31] and by Fermilab/MILC [41] both obtained values above the experimental average, although only by just over one standard deviation.

The result we present here is substantially more precise than these earlier studies and for the first time displays a significant, 6σ , difference from the experimental average, clearly showing that the lattice result lies above the experimental one. We interpret this as the effect of ignoring annihilation to gluons in the calculation of the η_c mass.

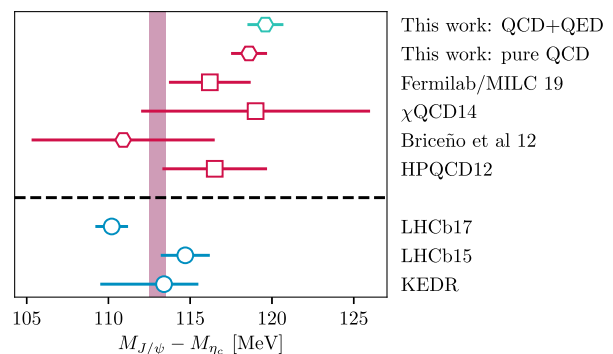


FIG. 9. Comparison of different lattice results for the charmonium hyperfine splitting and separate experimental results that measure this difference, as well as the PDG average (pink band). The PDG average is obtained from taking the differences of the PDG J/ψ and η_c masses (see Fig. 8) rather than only from experiments that directly measure the splitting. The squares give lattice QCD results from calculations that include $n_f = 2 + 1$ flavors of quarks in the sea. The hexagons give results that include $n_f = 2 + 1 + 1$ flavors of sea quarks, including the results we present here at the top of the plot. All lattice QCD results have had uncertainties from neglecting η_c annihilation removed so that we might expect some difference between them and experiment (see text), but previous lattice QCD results have not been accurate enough to see this. The Fermilab/MILC result used Fermilab c quarks on gluon field configurations with asqtad-sea quarks [41] and the previous HPQCD result [31] used HISQ quarks on the same asqtad-sea ensembles. Briceño *et al.* [42] used a modification of the Fermilab approach known as relativistic heavy quarks on the $n_f = 2 + 1 + 1$ HISQ sea-quark ensembles that we use here. The χ QCD result [43] used overlap quarks on gluon field configurations including $n_f = 2 + 1$ domain-wall sea quarks.

From the comparison of our results to experiment we conclude that these annihilation effects increase the η_c mass by 7.3(1.2) MeV, where the uncertainty is dominated by that from the lattice calculation.

Previous analyses of this issue have given mixed results. In NRQCD perturbation theory [8] we can relate the shift in the η_c mass to its total (hadronic) width through the perturbative amplitude for $c\bar{c} \rightarrow gg \rightarrow c\bar{c}$ at threshold [44]. Then

$$\begin{aligned} \Delta M_{\eta_c} &= \frac{\Gamma_{\eta_c}}{2} \left(\frac{2(\ln 2 - 1)}{\pi} + \mathcal{O}(\alpha_s, v^2/c^2) \right) \\ &= \frac{31.9(7)}{2} \text{MeV} \times (-0.195 + \mathcal{O}(\alpha_s, v^2/c^2)). \end{aligned} \quad (11)$$

The leading term here gives -3.1 MeV, but subleading corrections could easily change the sign. An alternative way to think about the effect is nonperturbatively and then the gluon annihilation allows mixing between the η_c and other flavor-singlet pseudoscalar mesons. Since these are lighter than the η_c this mixing could give a positive correction to the η_c mass. Direct lattice QCD determination of the effect, by calculating the appropriate quark-line disconnected correlation functions, has so far not proved possible. This is because the lighter states that are introduced by the mixing make it very hard to pin down a small effect on the mass of a particle, the η_c , which is so much further up the spectrum in this channel. An estimate of the mass shift of $+1-4$ MeV was obtained in the quenched approximation in which this mixing is not possible but where mixing with glueballs could happen instead [45].

Our result for the hyperfine splitting, by its accuracy, provides for the first time a clear indication of the size of the impact of the η_c annihilation to gluons on its mass:

$$\Delta M_{\eta_c}^{\text{annihln}} = +7.3(1.2) \text{ MeV}. \quad (12)$$

IV. DETERMINATION OF m_c

A. Pure QCD

In [46] we showed that it is possible to determine the strange and charm quark masses accurately in lattice QCD using an intermediate momentum-subtraction scheme. By intermediate we mean that the mass renormalization factor to convert the tuned bare lattice quark mass to the momentum-subtraction scheme is calculated on the lattice. The conversion from the momentum subtraction to the final preferred $\overline{\text{MS}}$ scheme is carried out using QCD perturbation theory in the continuum. To do this accurately it is important to use a momentum-subtraction scheme that has only one momentum scale, μ . This means that the squared 4-momentum on each leg of the vertex diagram, from which the mass renormalization factor is calculated, is μ^2 . The RI-SMOM scheme [47] used in [46] is such a scheme. A further

important point is that the mass renormalization factor will be contaminated by nonperturbative (condensate) artifacts through its nonperturbative calculation on the lattice. To identify and remove these artifacts (that appear as inverse powers of μ) requires calculations at multiple values of μ and a fit to the results, as discussed in [46].

Below we briefly summarize the procedure followed in [46]:

- (1) Determine the tuned bare quark mass and lattice spacing at physical sea-quark masses for each set of gluon field configurations at a fixed β value. We do this following Appendix A of [26].
- (2) Calculate the mass renormalization factor, Z_m^{SMOM} , that converts the lattice quark masses to the RI-SMOM scheme for each β value at multiple values of μ . We thereby obtain the quark mass in the RI-SMOM scheme at scale μ .
- (3) Convert the mass to the $\overline{\text{MS}}$ scheme at scale μ using a perturbative continuum matching calculation. We denote this conversion factor by $Z_m^{\overline{\text{MS}}/\text{SMOM}}(\mu)$.
- (4) Run all the $\overline{\text{MS}}$ quark masses at a range of scales μ to a reference scale of 3 GeV using the four loop QCD $\overline{\text{MS}}$ β function. We denote these running factors $r(3 \text{ GeV}, \mu)$.
- (5) Fit all of the results for the $\overline{\text{MS}}$ mass at 3 GeV to a function that allows for discretization effects and condensate contamination, which begins at $1/\mu^2$ with the non-gauge-invariant $\langle A^2 \rangle$ condensate.
- (6) Obtain from the fit the physical value for the quark mass in the $\overline{\text{MS}}$ scheme at 3 GeV with condensate contamination removed.

Here we provide three small updates to [46]. We first list them and then discuss them in more detail below. The three updates are

- (1) we improve the uncertainty in the tuning of the bare lattice c -quark mass by using the J/ψ mass rather than the η_c ;
- (2) we include results from a finer ensemble of lattices (set 14) to provide even better control of the continuum limit;
- (3) we use the new 3-loop-accurate SMOM to $\overline{\text{MS}}$ matching factors, $Z_m^{\overline{\text{MS}}/\text{SMOM}}$, calculated in [48,49] to reduce the perturbative matching uncertainty.

The first update is to change how the tuning of the bare charm quark mass is done. In [46] bare charm masses were used that had been tuned to the experimental η_c mass, adjusted to allow for estimates of missing QED (from a Coulomb potential) and gluon annihilation effects (from perturbation theory). A 100% uncertainty was included on the adjustment [26]. Now that we are explicitly including quenched QED it makes more sense to have a tuning process that uses an experimental meson mass with no adjustments. We also want to use the same tuning process for both the pure QCD case and the QCD + QED case to allow for a clear comparison and one that reflects the

TABLE VI. Lattice spacing values and tuned c -quark masses at physical sea-quark masses for each group of ensembles at a fixed β value, denoted by their name in column 1 (see Table I). The lattice spacing value is given in units of w_0 in column 2 and the c quark mass, fixed from the J/ψ meson mass, is given in GeV units in column 3. The first uncertainty on the mass is uncorrelated between lattice spacing values, and the second is correlated.

| | w_0/a | m_c^{tuned} [GeV] |
|-----------|------------|----------------------------|
| Coarse | 1.4055(33) | 1.0524(10)(30) |
| Fine | 1.9484(33) | 0.9736(10)(30) |
| Superfine | 3.0130(56) | 0.8973(10)(30) |
| Ultrafine | 3.972(19) | 0.8592(20)(30) |

procedures that would be followed in a complete QCD + QED calculation. This means that we should use the J/ψ meson mass, as we have done in Sec. III. The J/ψ mass is more accurate experimentally than that of the η_c and the J/ψ has a much smaller width, implying little effect on the mass from its 3-gluon annihilation mode. The impact of J/ψ annihilation to a single photon is a sub-1 MeV shift to the mass which is a 0.02% effect, so negligible.

Using our J/ψ meson masses and following the procedure of [26] we obtain tuned bare c masses for each β value. These are given in Table VI along with the w_0/a values corresponding to physical sea-quark masses at that β value, which are also updated slightly from [46]. These slight changes in w_0/a lead to small adjustments in the μ values relative to those given in Table IV of [46]. This is accounted for when we run the Z_m to the correct reference scale in $\overline{\text{MS}}$.

The second update is to include results from the ultrafine $\beta = 7.0$ ensemble (set 14). The appropriate tuned mass and w_0/a value for physical sea-quark masses is given in Table VI. We have also calculated new $Z_m^{\text{SMOM}}(\mu)$ values on set 14. These are given in the Appendix.

The third update is to add the α_s^3 correction to the SMOM to $\overline{\text{MS}}$ conversion factor, $Z_m^{\overline{\text{MS}}/\text{SMOM}}$, for the mass renormalization. This correction was recently calculated in continuum perturbative QCD [48,49]. For $n_f = 4$, as here, the α_s^3 correction is a small effect (0.2%), continuing the picture seen at $\mathcal{O}(\alpha_s)$ and $\mathcal{O}(\alpha_s^2)$ and consistent with the uncertainty taken from missing it in [46].

Once we have determined results for $\bar{m}_c(3 \text{ GeV})$ at a variety of lattice spacing values using the SMOM intermediate scheme at a variety of μ values, we need to fit the results to determine $\bar{m}_c(3 \text{ GeV})$ in the continuum limit. We do this following our previous calculation [46], where the fit function is given in Eq. (26). The fit includes discretization effects and condensate artifacts in the lattice calculation of Z_m^{SMOM} . In [46] we included a term in the fit, $c_\alpha \alpha_s^3(\mu)$ (with α_s in the $\overline{\text{MS}}$ scheme) to allow for the then-missing α_s^3 term in the SMOM to $\overline{\text{MS}}$ conversion. Here we replace that term with $c_\alpha \alpha_s^4(\mu)$ since the conversion is now calculated through α_s^3 and included in our results. We

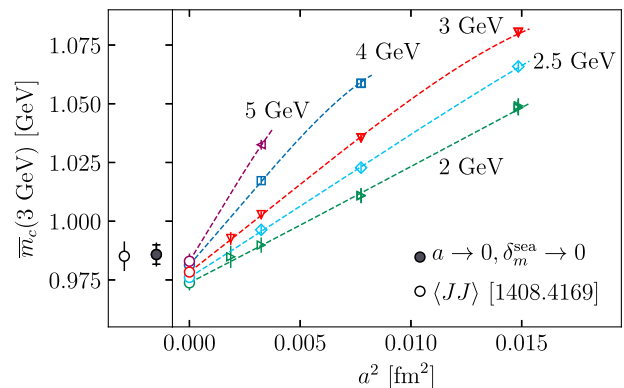


FIG. 10. $\bar{m}_c(3 \text{ GeV})$ extrapolated to the continuum with a fit form that allows for condensate terms that behave like inverse powers of the renormalization scale μ . This plot is an updated version of the upper section of Fig. 10 in [46], with added data points on ultrafine lattices (set 14) and a retuned bare c -quark mass fixed from the J/ψ , rather than η_c , meson. The ultrafine points have slightly mistuned μ values compared to the corresponding lines (see text).

take a prior value on c_α of 0.0 ± 0.5 . This allows for the coefficient of the α_s^4 -term in the conversion factor to be 4 times as large as the α_s^3 coefficient.

The updated fit to our results for \bar{m}_c in the $\overline{\text{MS}}$ scheme at 3 GeV is shown in Fig. 10. The fit has a $\chi^2/\text{d.o.f.}$ of 0.71. The error budget for this calculation is shown in Table VII. Most of the entries are very similar to those in [46]. The contribution due to the continuum extrapolation has, unsurprisingly, dropped a little, as has the uncertainty from the missing higher-order terms (here α_s^4) in the SMOM to $\overline{\text{MS}}$ conversion. The correlated tuning uncertainty comes largely from the uncertainty in the physical value of w_0 used to fix the lattice spacing. We will be able to reduce that uncertainty in the future by improving the determination of the value of w_0 .

Our updated pure QCD result is

$$\bar{m}_c(3 \text{ GeV})_{\text{QCD}} = 0.9858(51) \text{ GeV}. \quad (13)$$

Running this down to a scale equal to the mass gives

$$\bar{m}_c(\bar{m}_c)_{\text{QCD}} = 1.2723(78) \text{ GeV}. \quad (14)$$

These results improve on and supersede the value in [46].

B. Impact of quenched QED

To include quenched QED effects in the determination of the c -quark mass we must determine both the bare quark mass and the mass renormalization factor with quenched QED switched on.

We include quenched QED effects for Z_m in the RI-SMOM scheme in the same way as that described for the vector current renormalization in [16]. This involves the

TABLE VII. Error budget (in %) for the calculation of the charm quark mass in the $\overline{\text{MS}}$ scheme at a scale of 3 GeV using RI-SMOM as an intermediate scheme. The listed contributions have the same meaning as those in [46] except that we use r here for the running factor rather than R and we have an additional one labeled “QED effects” which comes from the continuum extrapolation shown in Fig. 12.

| | $\bar{m}_c(3 \text{ GeV})$ |
|--|----------------------------|
| $a^2 \rightarrow 0$ | 0.23 |
| Missing α_s^4 term | 0.10 |
| Condensate | 0.21 |
| m_{sea} effects | 0.00 |
| $Z_m^{\overline{\text{MS}}/\text{SMOM}}$ and r | 0.07 |
| Z_m^{SMOM} | 0.12 |
| Uncorrelated m^{tuned} | 0.15 |
| Correlated m^{tuned} | 0.30 |
| Gauge fixing | 0.09 |
| μ error from w_0 | 0.12 |
| QED effects | 0.02 |
| Total | 0.52 |

generation of U(1) fields in Landau gauge to remain consistent with the Landau gauge QCD configurations used in the pure QCD calculation. When converting from the RI-SMOM scheme for Z_m to the $\overline{\text{MS}}$ scheme it is also necessary to include QED effects in the perturbative matching factor. We can evaluate the QED contribution to $Z_m^{\overline{\text{MS}}/\text{SMOM}}$ at order α_{QED} by multiplying the known coefficient of α_s [47] by $(3/4)Q^2$ to give the coefficient of α_{QED} . The impact is very small ($<0.1\%$) and we therefore safely neglect higher order terms. The numerical values of the $\mathcal{O}(\alpha_{\text{QED}})$ -term we do include for the RI-SMOM to $\overline{\text{MS}}$ matching are given in Table VIII.

To assess the QED impact on the tuned bare c mass we use the QCD + QED J/ψ masses given in Table IV and shown in Fig. 2. As we have corrected the pure QCD determination of m_c to be tuned to the experimental J/ψ mass, this is the tuning we will use for the QCD + QED case as well. The fractional shift in am_c required to obtain the correct J/ψ mass after QED has been included (which we denote $R_{\text{QED}}[am_c]$) can be evaluated from the fractional change in the J/ψ mass. $R_{\text{QED}}[am_c]$ is the fractional change in am_c required to return the J/ψ mass to the value it had in pure QCD (i.e., the experimental value) once QED is switched on. Thus the increase in J/ψ mass seen with QED must be compensated by a corresponding reduction in am_c . From the deliberately mistuned am_c values in Table III we see that the fractional change in the c mass is 1.5 times larger than the change seen in the meson mass. We can use this factor, along with $R_{\text{QED}}^0[M_{J/\psi}]$ values from Table IV and the required change of sign in the shift, to determine the retuning of the quark masses in QCD + QED. We therefore take $R_{\text{QED}}[am_c]$ on coarse, fine and superfine lattices (sets

TABLE VIII. Table giving factors needed for the determination of the quark mass in a calculation including quenched QED for different μ values and lattice spacings (denoted by set numbers). The fractional QED correction to Z_m^{SMOM} is given in the third column, the QED component of the RI-SMOM to $\overline{\text{MS}}$ matching for each μ in the fourth column and the factor giving the QED mass running from μ to a reference scale of 3 GeV in the fifth column.

| Set | μ [GeV] | $R_{\text{QED}}[Z_m^{\text{SMOM}}]$ | $Z_m^{\overline{\text{MS}}/\text{SMOM}}_{\text{QED}}$ | $r^{\text{QED}}(3 \text{ GeV}, \mu)$ |
|-----|-------------|-------------------------------------|---|--------------------------------------|
| 5 | 2 | 1.001200(83) | 0.999872 | 0.999372 |
| 10 | 2 | 1.001516(35) | 0.999872 | 0.999372 |
| 12 | 2 | 1.001853(83) | 0.999872 | 0.999372 |
| 5 | 2.5 | 1.000827(31) | 0.999873 | 0.999718 |
| 5 | 3 | 1.000540(15) | 0.999873 | ... |
| 10 | 3 | 1.000851(11) | 0.999873 | ... |
| 12 | 3 | 1.001308(18) | 0.999873 | ... |
| 10 | 4 | 1.0005001(21) | 0.999873 | 1.000446 |
| 12 | 4 | 1.0009331(34) | 0.999873 | 1.000446 |

6, 10 and 12) to be 0.99840(8), 0.99790(4) and 0.99734(9) respectively. We increase the uncertainty on $R_{\text{QED}}[am_c]$ compared to that for $R_{\text{QED}}^0[M_{J/\psi}]$ by a factor of 5 to allow for the uncertainty in our conversion factor of 1.5 above.

We calculate the ratio of Z_m in the SMOM scheme in QCD + QED to pure QCD ($R_{\text{QED}}[Z_m^{\text{SMOM}}]$) following the methods of [46]. The calculations are carried out at multiple values of the renormalization scale μ and extrapolated to zero valence quark mass. Results are given in Table VIII. Notice that these values are larger than 1 and so compensate to a large extent for the changes in the tuning of the bare lattice am_c induced by QED. This reflects the fact that most of the shift is an unphysical ultraviolet self-energy effect. We then convert from the SMOM scheme to $\overline{\text{MS}}$ by making use of the ratio of the perturbative conversion factor for QCD + QED to pure QCD, i.e., the $\mathcal{O}(\alpha_{\text{QED}})$ piece of $Z_m^{\overline{\text{MS}}/\text{SMOM}}$ also given in Table VIII. This is less than 1 but only by a very small amount.

Multiplying these two factors together gives the ratio of the lattice to $\overline{\text{MS}}$ mass renormalization factors for QCD + QED to that for pure QCD, i.e., $R_{\text{QED}}[Z_m^{\overline{\text{MS}}}]$. From Table VIII, multiplying columns 3 and 4, we can see that $R_{\text{QED}}[Z_m^{\overline{\text{MS}}}]$ varies with μ and with lattice spacing over a range of about 0.001. In perturbation theory we expect $R_{\text{QED}}[Z_m^{\overline{\text{MS}}}]$ to consist of a power series in α_{QED} and α_s , multiplied by constants and powers of logarithms of $a\mu$. The leading logarithm at each order can be derived from the anomalous dimensions of the mass, allowing us to write [50]

$$R_{\text{QED}}[Z_m^{\overline{\text{MS}}}] = 1 + C_m - \frac{3\alpha_{\text{QED}}Q^2}{4\pi} \log(\mu^2 a^2). \quad (15)$$

Here C_m is a constant, up to discretization effects and higher-order terms multiplying powers of $\log(a\mu)$. Figure 11 plots our results for C_m . These show very little variation with a and μ , confirming that the dependence on a and μ of $R_{\text{QED}}[Z_m^{\overline{\text{MS}}}]$ is almost entirely captured by Eq. (15).

Once the impact of QED on the c mass in the $\overline{\text{MS}}$ scheme at scale μ is obtained, as above, we then need to allow for QED effects in the running of the masses from μ to the reference scale of 3 GeV. This is done by multiplication by a factor r^{QED} calculated in $\mathcal{O}(\alpha_{\text{QED}})$ perturbation theory and given in Table VIII. These numbers are also very close to 1. The $\alpha_s \alpha_{\text{QED}}$ term could in principle have some impact here but it is very small and we neglect it [50].

Multiplying $R_{\text{QED}}[am_c]$ and $R_{\text{QED}}[Z_m^{\overline{\text{MS}}}]$ together allows us to determine the ratio of the c -quark mass in the $\overline{\text{MS}}$ scheme at 3 GeV from QCD + QED to that in pure QCD, i.e., $R_{\text{QED}}[\bar{m}_c(3 \text{ GeV})]$. The values that we have for this ratio come from results at multiple values of μ and multiple values of the lattice spacing. To determine the physical ratio in the continuum limit with condensate contamination removed (in this case QED corrections to QCD condensates) we need to fit the results to a similar form to that used in [46]. We use

$$\begin{aligned}
R_{\text{QED}}[\bar{m}_c(3 \text{ GeV}, \mu, a)] &= R_{\text{QED}}[\bar{m}_c(3 \text{ GeV})] \\
&\times \left[1 + \alpha_{\text{QED}} Q^2 \sum_{i=1} c_a^{(i)} (a(1 \text{ GeV}))^{2i} \right] \\
&\times \left[1 + \alpha_{\text{QED}} Q^2 \left(\sum_{j=1} c_{\mu^2 a^2}^{(j)} (a\mu)^{2j} \right. \right. \\
&\left. \left. + \sum_{n=1} \alpha_s(\mu) c_{\text{cond}}^{(n)} \frac{(1 \text{ GeV})^{2n}}{\mu^{2n}} \right) \right]. \quad (16)
\end{aligned}$$

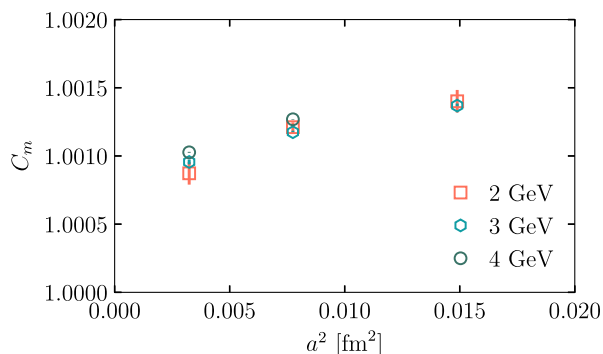


FIG. 11. The factor C_m that forms part of the QED effect in the lattice to $\overline{\text{MS}}$ mass renormalization, as defined in Eq. (15), plotted against the square of the lattice spacing. The fact that C_m , as shown here, has almost no μ or a dependence demonstrates that the μa dependence seen in $R_{\text{QED}}[Z_m^{\overline{\text{MS}}}]$ from columns 3 and 4 of Table VIII is simply that expected from perturbation theory.

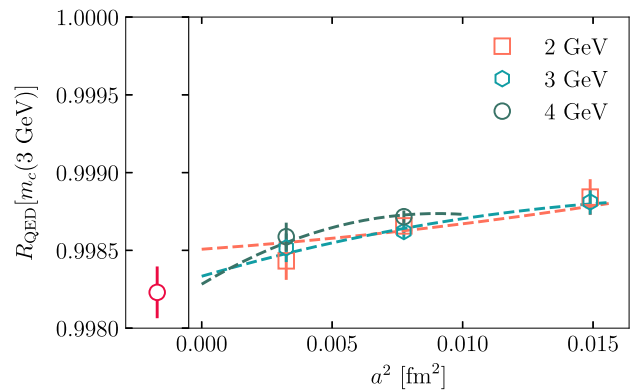


FIG. 12. QED correction to the charm quark mass in the $\overline{\text{MS}}$ scheme at a scale of 3 GeV. The different μ values, shown as different colors and shapes, have all been run to 3 GeV and only differ by discretization and condensate effects. The red point on the left is the result for $R_{\text{QED}}[\bar{m}_c(3 \text{ GeV})]$ returned by the fit of Eq. (16).

The first term on the second line of Eq. (16) accounts for discretization effects in $R_{\text{QED}}[am_c]$; a scale of 1 GeV is chosen in these effects as this is close to the c -quark mass. The term multiplying this (on the bottom two lines) models the a and μ dependence of the QED correction to Z_m . This includes discretization effects of the form $(a\mu)^{2i}$ and terms to model condensate contributions, starting at $1/\mu^2$. The priors on all coefficients are taken as 0.0 ± 1.0 , except for the physical result, $R_{\text{QED}}[\bar{m}_c(3 \text{ GeV})]$, for which we take prior 1.00(1).

The lattice QCD results for $R_{\text{QED}}[\bar{m}_c(3 \text{ GeV})]$ and the fit output are shown in Fig. 12. The fit has a $\chi^2/\text{d.o.f.}$ of 0.87 and returns a physical value of $R_{\text{QED}}[\bar{m}_c(3 \text{ GeV})]$ of 0.99823(17). We conclude that the impact of quenched QED is to lower the c -quark mass, $\bar{m}_c(3 \text{ GeV})$ by a tiny amount: 0.18(2)%.

We obtain our final answer for the c quark mass in QCD + QED by multiplying $R_{\text{QED}}[\bar{m}_c(3 \text{ GeV})]$ by our pure QCD result for $\bar{m}_c(3 \text{ GeV})$. This gives the QCD + QED result of

$$\bar{m}_c(3 \text{ GeV})_{\text{QCD+QED}} = 0.9841(51) \text{ GeV}. \quad (17)$$

Running down to the scale of the mass with QCD + QED gives

$$\bar{m}_c(\bar{m}_c)_{\text{QCD+QED}} = 1.2719(78) \text{ GeV}, \quad (18)$$

very close to the pure QCD value at this scale. This is the first determination of the c -quark mass to include QED effects explicitly, rather than estimate them phenomenologically as has been done in the past. The uncertainty achieved here of 0.5% is smaller than the 0.6% from [46] because we have reduced several sources of uncertainty, mainly those from the extrapolation to the continuum limit

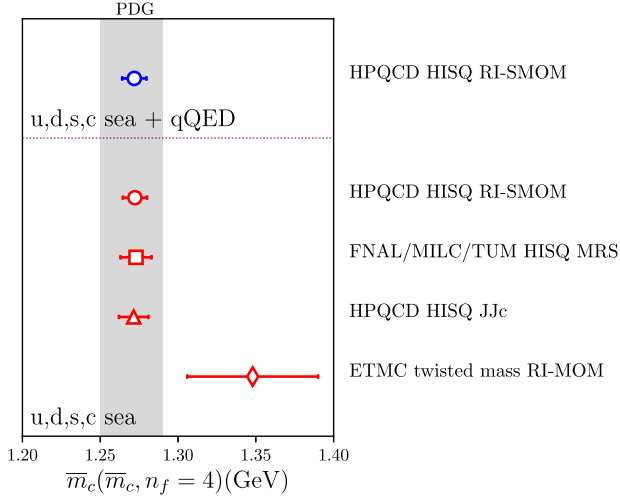


FIG. 13. Comparison of lattice QCD results for m_c that include u , d , s and c quarks in the sea. The top two results are the ones from this paper. Our QCD + quenched QED result is given in Eq. (17). Our pure QCD result, Eq. (13), supersedes our earlier result in [46]. The Fermilab/MILC/TUM result is from [51] and uses a method based on charm-light meson masses. The “HPQCD HISQ JJe” result is from [26] and uses current-current correlator techniques. These three results agree to better than 1%. The ETMC result is from [52] and uses the RI-MOM intermediate scheme. The grey band gives the $\pm 1\sigma$ uncertainty band from the Particle Data Group [1].

and from missing higher-order terms in the SMOM to $\overline{\text{MS}}$ matching.

C. Discussion: m_c

Figure 13 gives a comparison of lattice QCD results for \overline{m}_c . We plot the masses at the scale of the mass, as is conventional even though this is a rather low scale. We restrict the comparison to results that were obtained on gluon field configurations including u , d , s and c quarks in the sea. The top result is our value from Eq. (17) that explicitly includes a calculation of the impact of quenched QED on the determination of the quark mass.

The top three results in the pure QCD section of the figure all include an estimate of, and correction for, QED effects. These corrections are made, however, by allowing for “physical” QED effects such as those arising from the Coulomb interaction between quark and antiquark in a meson. They do not allow for the QED self-energy contribution which is substantial. Although a large part of this is canceled by the impact of QED on the mass renormalization, a consistent calculation has to include both effects, as we have done here.

An important point about Fig. 13 is that the top three pure QCD results all have uncertainties of less than 1% and agree to better than 1%, using completely different methods. This implies a smaller uncertainty on \overline{m}_c than the 1.5% allowed for by the Particle Data Group [1]. This impressive

agreement is not changed by our new result including quenched QED because, as we have shown, the impact of this is at the 0.2% level.

V. J/ψ AND η_c DECAY CONSTANTS

The decay constant of the J/ψ , $f_{J/\psi}$, is defined from the matrix element between the vacuum and a J/ψ meson at rest by

$$\langle 0 | \bar{\psi} \gamma_\mu \psi | J/\psi \rangle = f_{J/\psi} M_{J/\psi} \epsilon_\mu, \quad (19)$$

where ϵ_μ is the component of the polarization of the J/ψ in the direction of the vector current. In terms of the ground-state amplitude, A_0^V , and mass, M_0^V ($\equiv E_0^V$), obtained from the fit of Eq. (3) to the charmonium vector correlator it is (in lattice units)

$$f_{J/\psi} = Z_V \sqrt{\frac{2A_0^V}{M_0^V}}. \quad (20)$$

Z_V is the renormalization factor required to match the lattice vector current to that in continuum QCD if a nonconserved lattice vector current is used (as here). We discuss the renormalization of vector currents using intermediate momentum-subtraction schemes in [16] and we will make use of the results based on the RI-SMOM scheme here (see Sec. II). Note that there is no additional renormalization required to get from the RI-SMOM scheme to $\overline{\text{MS}}$ because the RI-SMOM scheme satisfies the Ward-Takahashi identity [16].

The partial decay width of the J/ψ to an $\ell^+ \ell^-$ pair ($\ell = e, \mu$) is directly related to the decay constant. At leading order in α_{QED} and ignoring $(m_\ell/M_{J/\psi})^4$ correction terms, the relation is

$$\Gamma(J/\psi \rightarrow \ell^+ \ell^-) = \frac{4\pi}{3} \alpha_{\text{QED,eff}}^2 (M_{J/\psi}^2) Q_c^2 \frac{f_{J/\psi}^2}{M_{J/\psi}}, \quad (21)$$

where Q_c is the electric charge of the charm quark in units of the charge of the proton. Note that the formula contains the effective coupling, $\alpha_{\text{QED,eff}}$ evaluated at the scale of $M_{J/\psi}$ but without including the effect of the J/ψ resonance in the running of α_{QED} to avoid double counting [53].

Experimental values of $\Gamma(J/\psi \rightarrow e^+ e^-)$ are obtained by mapping out the cross section for $e^+ e^- \rightarrow e^+ e^-$ and $e^+ e^- \rightarrow$ hadrons through the resonance region [54] or by using initial-state radiation to map out this region via $e^+ e^- \rightarrow \mu^+ \mu^- \gamma$ [55]. In either case initial-state radiation and nonresonant background must be taken care of [56,57]. A cross section fully inclusive of final-state radiation is obtained; interference between initial- and final-state radiation is heavily suppressed [58]. The resonance parameter determined by the experiment is then the “full” partial width [57,59],

$$\Gamma_{\ell\ell} = \frac{\Gamma_{\ell\ell}^{(0)}}{|1 - \Pi_0|^2} \quad (22)$$

where $\Gamma^{(0)}$ is the partial width to lowest order in QED and Π_0 is the photon vacuum polarization. The effect of the vacuum polarization is simply to replace α_{QED} in the lowest-order QED formula for the width with $\alpha_{\text{QED,eff}}(M^2)$, as we have done in Eq. (21).

The experimental determination of $\Gamma_{\ell\ell}$ is accurate to 2% for the J/ψ [1]. This allows us to infer a decay constant value from experiment, accurate to 1%, using Eq. (21).

$$\begin{aligned} f_{J/\psi}^{\text{expt}} &= \left(\frac{3M_{J/\psi}}{4\pi Q_c^2} \right)^{1/2} \frac{\Gamma_{e^+e^-}^{1/2}}{\alpha_{\text{QED,eff}}} \\ &= 40.786(\text{MeV})^{1/2} \frac{\Gamma_{e^+e^-}^{1/2}}{\alpha_{\text{QED,eff}}}. \end{aligned} \quad (23)$$

Using the experimental average of $\Gamma_{e^+e^-} = 5.53(10)$ keV [1] and $\alpha_{\text{QED,eff}}(M_{J/\psi}^2) = 1/134.02(3)$ [60] gives

$$f_{J/\psi}^{\text{expt}} = 406.5(3.7)(0.5) \text{ MeV}. \quad (24)$$

The first uncertainty comes from the experimental uncertainty in Γ and the second is an $\mathcal{O}(\alpha_{\text{QED}}/\pi)$ uncertainty for higher order in QED terms, for example from final-state radiation, in the connection between Γ and f in Eq. (21). Note that using α_{QED} of 1/137 would increase this number by 2.3% (9 MeV).

This experimental value can then be compared to our lattice QCD results for a precision test of QCD. Here we improve on HPQCD's earlier calculation [31] by working on gluon field configurations that cover a wider range of lattice spacing values and with sea u/d quark masses now down to their physical values. In addition we now include c quarks in the sea and have a more accurate determination of the vector renormalization factor Z_V [16]. We will also test the impact on $f_{J/\psi}$ of the c quark's electric charge.

The decay constant of the pseudoscalar η_c meson is determined from our pseudoscalar correlators (of spin-taste $\gamma_5 \otimes \gamma_5$) using the ground-state mass and amplitude parameters from the correlator fit, Eq. (2):

$$f_{\eta_c} = 2m_c \sqrt{\frac{2A_0^P}{(M_0^P)^3}}. \quad (25)$$

Note that this is absolutely normalized and no Z factor is required. Because the η_c does not annihilate to a single particle there is no experimental process from which we can directly determine f_{η_c} . Nevertheless it is a useful quantity to calculate for comparison to $f_{J/\psi}$ and to fill out the picture of these hadronic parameters from lattice QCD [61]. Again we will improve on HPQCD's earlier calculation [62] as discussed above for the J/ψ .

A. Pure QCD

The second column of Table IX gives our results for the (un-normalized) values of $af_{J/\psi}$ in pure QCD on 12 of the

TABLE IX. Columns 2 and 3 give the results in lattice units for the J/ψ and η_c decay constants respectively in pure QCD on the ensembles listed in Table I. The values of am_c^{val} are those given in Table I except for two cases with a deliberately mistuned c -quark mass: set 6 denoted by a * where $am_c = 0.643$ and set 14 denoted by a † where $am_c = 0.188$. The results for $f_{J/\psi}$ do not include the multiplication by Z_V needed to normalize them [Eq. (20)]. Columns 4 and 5 give the electromagnetic corrections for the J/ψ and η_c decay constants, as the ratio of the QCD + QED result to that in pure QCD. Again, the electromagnetic corrections for $f_{J/\psi}$ do not include the corrections to Z_V . Z_V values are given in Table X.

| Set | $af_{J/\psi}/Z_V$ | af_{η_c} | $R_{\text{QED}}^0[f_{J/\psi}/Z_V]$ | $R_{\text{QED}}^0[f_{\eta_c}]$ |
|-----|-------------------|---------------|------------------------------------|--------------------------------|
| 1 | 0.43370(55) | 0.37659(18) | ... | ... |
| 2 | 0.42346(48) | 0.370332(91) | 1.00410(64) | 1.00294(50) |
| 3 | 0.4163(11) | 0.366127(57) | ... | ... |
| 4 | 0.29411(21) | 0.268331(61) | ... | ... |
| 6 | 0.28835(15) | 0.263727(60) | 1.00341(37) | 1.00326(13) |
| 6* | 0.28671(15) | 0.262077(48) | ... | ... |
| 8 | 0.285592(88) | 0.261676(26) | ... | ... |
| 9 | 0.19406(30) | 0.18191(12) | ... | ... |
| 10 | 0.191341(79) | 0.179362(26) | 1.00295(12) | 1.002951(54) |
| 11 | 0.18961(15) | 0.178039(24) | ... | ... |
| 12 | 0.12334(10) | 0.117535(28) | 1.00283(33) | 1.00311(47) |
| 13 | 0.119606(63) | 0.114151(26) | ... | ... |
| 14 | 0.091380(85) | 0.087772(39) | ... | ... |
| 14† | 0.09069(29) | 0.086774(59) | ... | ... |

TABLE X. Vector current renormalization constants, $Z_V(\mu)$, using the RI-SMOM scheme at $\mu = 2$ GeV (column 2) and $\mu = 3$ GeV (column 3) in pure QCD for each β value corresponding to a group of ensembles in Table I. Column 4 gives the QED correction to Z_V at 2 GeV in the form of the ratio of the QCD + QED value to that of pure QCD. Most of these values are taken from [16] although the Z_V value at $\beta = 7$ and the QED correction at $\beta = 5.8$ are new here.

| β | $Z_V(2 \text{ GeV})$ | $Z_V(3 \text{ GeV})$ | $R_{\text{QED}}[Z_V(2 \text{ GeV})]$ |
|---------|----------------------|----------------------|--------------------------------------|
| 5.80 | 0.95932(18) | ... | 0.999544(14) |
| 6.00 | 0.97255(22) | 0.964328(75) | 0.999631(24) |
| 6.30 | 0.98445(11) | 0.977214(35) | 0.999756(32) |
| 6.72 | 0.99090(36) | 0.98702(11) | 0.999831(43) |
| 7.00 | 0.99203(108) | 0.99023(56) | ... |

sets from Table I. We multiply $af_{J/\psi}/Z_V$ by the value of Z_V and convert to physical units using the inverse lattice spacing. Z_V values are taken from [16] except for a new value calculated here for $\beta = 7.0$ (ultrafine) set 14. We collect these values in Table X. See the Appendix for a discussion of the Z_V results. The Z_V values are very precise and so have little impact on the uncertainty in $f_{J/\psi}$.

Our results for $f_{J/\psi}$ for the pure QCD case are shown in Fig. 14 plotted against the square of the lattice spacing (in units of the bare c -quark mass). Clear dependence on the lattice spacing is seen. This dependence comes from the amplitudes of the two-point correlators; the lattice spacing dependence of Z_V contributes very little to it. We also plot in Fig. 14 the results of the fit using Eq. (5). The priors for the fit are as given in Sec. II F with the prior on the physical value of $f_{J/\psi}$ [i.e., x in Eq. (5)] of 0.4(1). The $\chi^2/\text{d.o.f.}$ of the fit is 0.43. The agreement with the result derived from

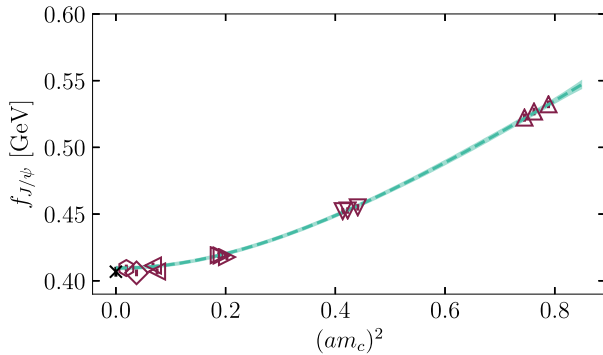


FIG. 14. The J/ψ decay constant calculated on the ensembles of Table I in pure QCD and plotted against the square of the bare c -quark mass in lattice units. The different red shapes correspond to different groups of ensembles with similar lattice spacing and the error bars shown include the full uncertainty on the points. Points at mistuned m_c are not plotted but are included in the fit. The green curve marks our extrapolation to the physical point, where the black cross shows the result determined from the experimental average for $\Gamma_{e^+e^-}$ from Eq. (24).

experiment can clearly be seen. We obtain an $f_{J/\psi}$ value in pure QCD of

$$f_{J/\psi,\text{QCD}} = 409.6(1.6) \text{ MeV}. \quad (26)$$

We will discuss this result further in Sec. V C.

We have used vector current renormalization factors, Z_V , in the RI-SMOM scheme at a scale of 2 GeV. The μ dependence of Z_V should just be the result of discretization effects and results for the physical quantity, $f_{J/\psi}$, using different renormalization scales μ should agree in the continuum limit. Here we verify that this is the case using $Z_V(2 \text{ GeV})$ and $Z_V(3 \text{ GeV})$ results from Table X [16]. There is no 3 GeV result on the very coarse lattices since μa would be too large. The comparison for $f_{J/\psi}$ using $\mu = 2$ and 3 GeV is shown in Fig. 15 for the pure QCD case. The difference between the two values of μ is barely visible. The values at $\mu = 3$ GeV give a continuum limit result of $f_{J/\psi} = 408.7(1.8) \text{ MeV}$, in good agreement with that at $\mu = 2$ GeV in Eq. (26) but slightly less accurate. The $\chi^2/\text{d.o.f.}$ of the fit was 0.45.

Our results for af_{η_c} , the η_c decay constant in lattice units, are given in the third column of Table IX for the pure QCD case. After conversion to physical units, they are plotted in Fig. 16. The curve is similar to that for $f_{J/\psi}$ but with somewhat smaller discretization effects. We also plot the results of performing the same fit as for $f_{J/\psi}$ using Eq. (5). The $\chi^2/\text{d.o.f.}$ of the fit is 0.88 giving a result for the decay constant in pure QCD of

$$f_{\eta_c,\text{QCD}} = 397.5(1.0) \text{ MeV}. \quad (27)$$

This agrees well with the earlier HPQCD value on $n_f = 2 + 1$ gluon field configurations [62] of 0.3947(24) GeV but has half the uncertainty. In [62] the effects from neglecting the charm quark in the sea are estimated to

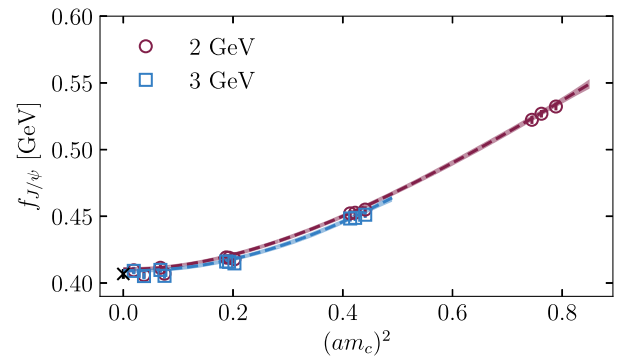


FIG. 15. The continuum extrapolation of $f_{J/\psi}$ using $Z_V(2 \text{ GeV})$ (results and fit curve in red, same values as in Fig. 14) and $Z_V(3 \text{ GeV})$ (results and fit curve in blue). The continuum extrapolated results agree in the two cases as they should. A black cross shows the experimental average result from Eq. (24).

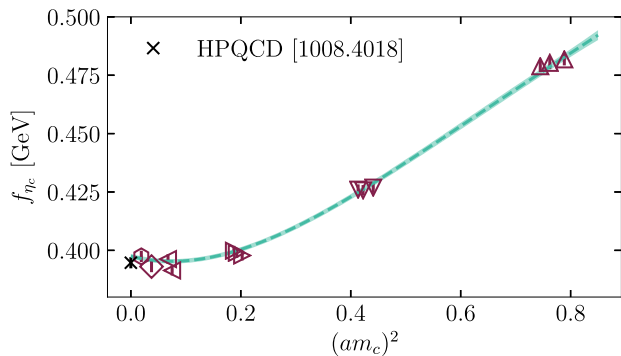


FIG. 16. The η_c decay constant calculated on the ensembles of Table I in pure QCD and plotted against the square of the bare c -quark mass in lattice units. The different red shapes correspond to different groups of gluon field ensembles with similar lattice spacing. The error bars on each point are the full uncertainty, including correlated uncertainties from, for example, the determination of the lattice spacing. The green curve shows our fit and extrapolation to the physical point. The black cross gives the earlier HPQCD result on $n_f = 2 + 1$ gluon field configurations from [62].

be $\mathcal{O}(0.01\%)$ which is negligible and means that the two calculations should give the same result.

Figure 17 shows our results for the ratio of $f_{J/\psi}$ to f_{η_c} in pure QCD. A lot of the discretization effects cancel in the ratio, as is evident in comparing this figure to Figs. 14 and 16. Systematic uncertainties, for example from the determination of the lattice spacing, are also reduced. The shape of the curve again, as in the hyperfine splitting case, reflects the fact that we have successfully reduced sources of a^2 error to the point where a^4 and a^6 are visible.

We fit the ratio to the same fit as before [Eq. (5)] with a prior on the physical value of 1.0(1). The fit has a $\chi^2/\text{d.o.f.}$

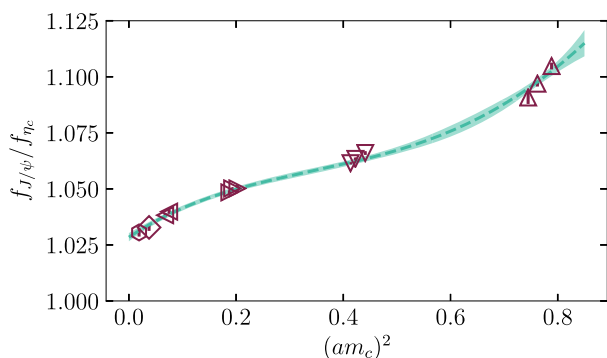


FIG. 17. The ratio of J/ψ to η_c decay constant determined in pure QCD, plotted against the square of the bare c -quark mass in lattice units. The different red shapes correspond to different groups of gluon field ensembles with similar lattice spacing. The error bars on each point are the full uncertainty, including correlated uncertainties from, for example, the determination of the lattice spacing. The green curve shows our fit and extrapolation to the physical point.

TABLE XI. Error budget for the J/ψ and η_c decay constants as a percentage of the final answer.

| | $f_{J/\psi}$ | f_{η_c} |
|----------------------|--------------|--------------|
| $a^2 \rightarrow 0$ | 0.09 | 0.03 |
| Z_V | 0.05 | ... |
| Pure QCD statistics | 0.12 | 0.05 |
| QCD + QED statistics | 0.05 | 0.02 |
| w_0/a | 0.11 | 0.08 |
| w_0 | 0.34 | 0.24 |
| Valence mistuning | 0.05 | 0.01 |
| Sea mistuning | 0.01 | 0.00 |
| Total | 0.40% | 0.26% |

of 0.62 and returns a physical value for the decay constant ratio in pure QCD of

$$\frac{f_{J/\psi, \text{QCD}}}{f_{\eta_c, \text{QCD}}} = 1.0285(18). \quad (28)$$

Thus we see that the J/ψ decay constant is nearly 3% larger than that of the η_c with an uncertainty of 0.2%.

Table XI gives the error budget for our final values of $f_{J/\psi}$ and f_{η_c} , both for the pure QCD case and the QCD + QED case to be discussed in Sec. VB. The contributions from different sources are very similar between the two decay constants. It is clear from this that the dominant sources of error are related to the determination of the lattice spacing, as for the hyperfine splitting.

The error budget presented here for the J/ψ decay constant is markedly different from that of [31]. There the dominant contribution to the error was from the vector renormalization constant, Z_V , obtained using a matching between lattice time moments and high order perturbative QCD [63]. Here that error is substantially reduced by using the Z_V values obtained in lattice QCD fully nonperturbatively in the RI-SMOM scheme [16]. Note that the uncertainty from scale setting in the decay constant is much smaller than that for the hyperfine splitting (Table V). This is because the decay constant has opposite behavior as a function of quark mass, increasing as the quark mass increases rather than decreasing. This then offsets, rather than augments (as in the hyperfine splitting case), its sensitivity to changes in the scale-setting parameter, w_0 .

B. Impact of quenched QED

Including quenched QED effects into our calculations allows us to determine the effect on the J/ψ and η_c decay constants of the electric charge of the valence c quarks. Because the J/ψ and η_c are electrically neutral particles, there is no long-distance infrared component to cause problems (as there is for f_{π^+}) and we can simply proceed to determine the decay constants after the addition of the QED field as we did in the pure QCD case.

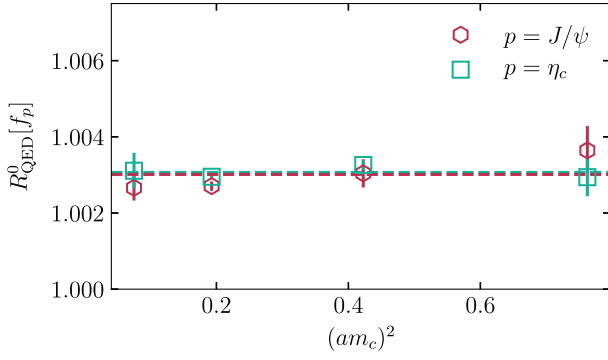


FIG. 18. The fractional QED correction to the J/ψ and η_c decay constants as a function of lattice spacing. The horizontal dashed lines mark the weighted average of the points.

The fractional QED effect on the J/ψ and η_c decay constants at fixed bare c -quark mass in lattice units is given in Table IX. We see a 0.3% increase, offset slightly by the change in Z_V in the J/ψ case. The fractional QED effect on Z_V is given in Table X. The fractional QED effect at fixed bare mass is plotted in Fig. 18. We see that the effect is similar for the J/ψ and η_c in the continuum limit and shows very little dependence on the lattice spacing.

The volume dependence of the fractional QED effect is shown in Fig. 19 on sets 5–7. We find that the effect is negligible well below the 0.1% level.

We now combine our QCD + QED results with our pure QCD results and the full fit of Eq. (5), which takes into account the retuning of the quark mass needed when quenched QED is included. Figure 20 shows our pure QCD results, QCD + QED results and fit curve for the J/ψ decay constant. We obtain

$$f_{J/\psi, \text{QCD+QED}} = 410.4(1.7) \text{ MeV}. \quad (29)$$

This is a 0.2% increase over the value in pure QCD [Eq. (26)] because retuning reduces the quark mass and offsets some of the impact of quenched QED seen in

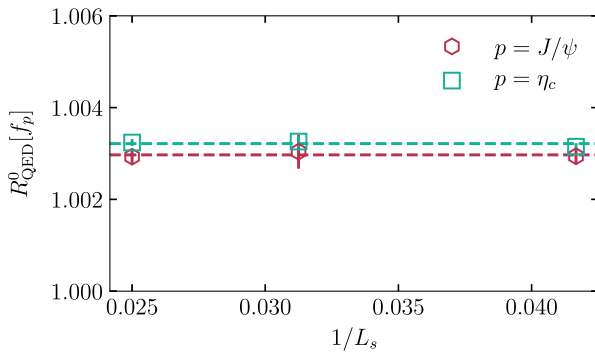


FIG. 19. The volume dependence of the fractional QED effect on the J/ψ and η_c decay constants measured on sets 5–7. The dashed lines are horizontal and indicate the weighted average of the points. There is no observable finite-volume effect at the level of our statistical uncertainties.

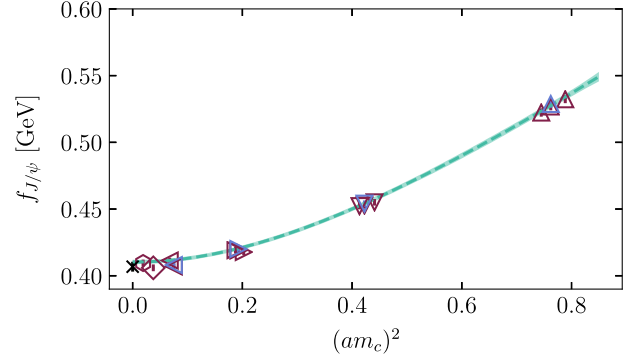


FIG. 20. The J/ψ decay constant calculated on the ensembles of Table I in pure QCD (red points) and including also quenched QED (blue points) plotted against the square of the bare c -quark mass in lattice units. The green curve marks our extrapolation to the physical point, where the black cross shows the experimental average result from Eq. (24).

Table IX. A more accurate statement is that the final fractional effect from quenched QED is $R_{\text{QED}}[f_{J/\psi}] = 1.00188(36)$.

A very similar picture is seen for f_{η_c} in Fig. 21. We obtain

$$f_{\eta_c, \text{QCD+QED}} = 398.1(1.0) \text{ MeV}. \quad (30)$$

The final fractional effect from quenched QED is then $R_{\text{QED}}[f_{\eta_c}] = 1.00166(25)$.

Finally, in Fig. 22 we plot results for the ratio of J/ψ to η_c decay constants and show the fit curve extrapolated to the continuum limit. This gives

$$\frac{f_{J/\psi, \text{QCD+QED}}}{f_{\eta_c, \text{QCD+QED}}} = 1.0284(19). \quad (31)$$

This is almost the same as the pure QCD result.

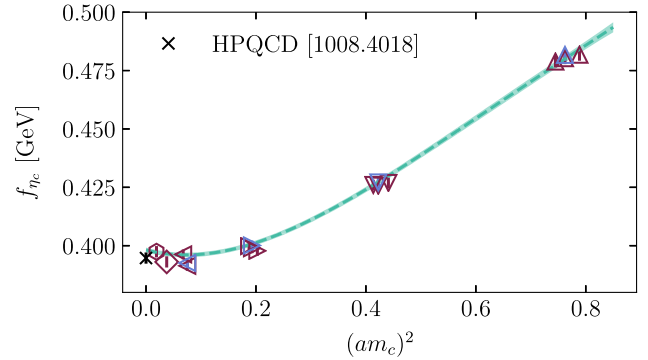


FIG. 21. The η_c decay constant calculated on the ensembles of Table I in pure QCD (red points) and including also quenched QED (blue points) plotted against the square of the bare c -quark mass in lattice units. The green curve marks our extrapolation to the physical point. The black cross gives the earlier HPQCD result on $n_f = 2 + 1$ gluon field configurations from [62].

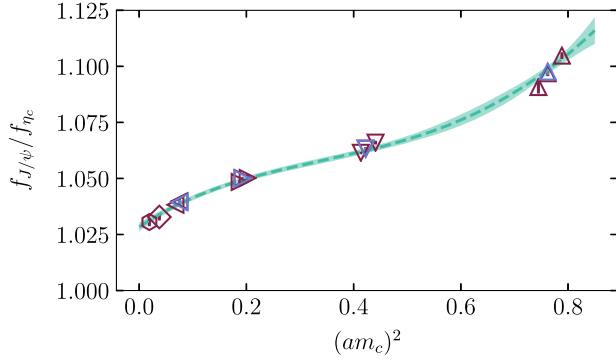


FIG. 22. The ratio of J/ψ to η_c decay constants calculated on the ensembles of Table I in pure QCD (red points) and including also quenched QED (blue points) plotted against the square of the bare c -quark mass in lattice units. The green curve marks our extrapolation to the physical point.

C. Discussion: $f_{J/\psi}$ and f_{η_c}

Figure 23 compares our new pure QCD and QCD + QED results to previous results including $n_f = 2 + 1$ flavors of sea quarks for f_{η_c} [62] and $f_{J/\psi}$ [31]. There is good agreement. These earlier calculations also used HISQ quarks but our new results are more accurate, particularly for $f_{J/\psi}$ because of the use of more accurate values of Z_V [16].

There have also been calculations that use $n_f = 2$ flavors of sea quarks. It is harder to make a comparison to these results because it is not clear what the systematic error is from not including at least the s quarks in the sea, and no uncertainty is included for this. The calculation of [64] uses twisted-mass quarks on $n_f = 2$ gluon field configurations and obtains $f_{\eta_c} = 387(7)(2)$ MeV and $f_{J/\psi} = 418(8)(5)$ MeV. The calculation of [65] uses clover quarks on $n_f = 2$ CLS gluon-field configurations to give $f_{\eta_c} = 387(3)(3)$ MeV and $f_{J/\psi} = 399(4)(2)$ MeV. The $n_f = 2$ results for f_{η_c} agree with each other and have a central value about 2σ below ours. The σ here is that from the $n_f = 2$ results since our uncertainty is much smaller. The $n_f = 2$ results for $f_{J/\psi}$ are compatible with each other and with our result, again at 2σ .

As discussed in Sec. V, the J/ψ decay constant is the hadronic quantity that is needed to determine the rate of J/ψ annihilation to leptons via Eq. (21). Our result for Γ using Eq. (21) with $f_{J/\psi}$ from Eq. (29) is

$$\Gamma(J/\psi \rightarrow e^+e^-) = 5.637(47)(13) \text{ keV}. \quad (32)$$

The first uncertainty is from our lattice QCD + QED result for $f_{J/\psi}$ and the second uncertainty allows for a relative $\mathcal{O}(\alpha_{\text{QED}}/\pi)$ correction to Eq. (21) from higher-order effects.

Figure 24 compares this width $\Gamma(J/\psi \rightarrow e^+e^-)$ to results from experiment. Recent experimental results from KEDR [54] and BES III [55] are shown along with the

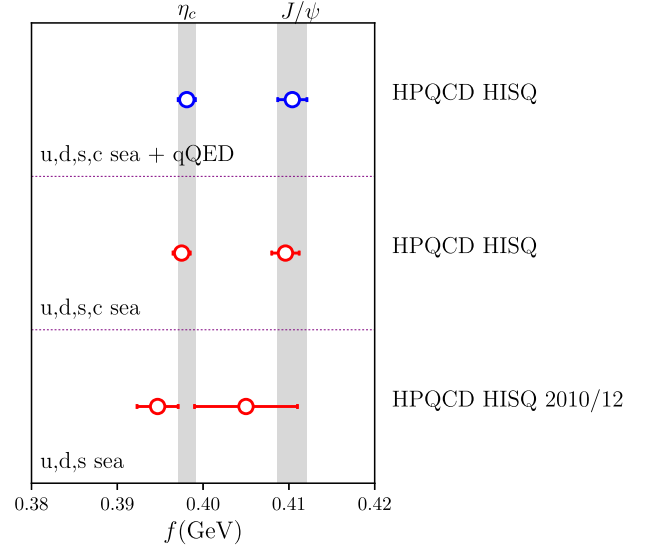


FIG. 23. A comparison of our new results for f_{η_c} and $f_{J/\psi}$ with earlier lattice QCD results, also by HPQCD, on gluon field configurations that include $n_f = 2 + 1$ flavors of quarks in the sea. The results labeled “HPQCD HISQ” are from this paper and the results labeled “HPQCD HISQ 2010/12” are from [31,62]. The grey bands are the $\pm 1\sigma$ bands from our new QCD + QED results.

Particle Data Group average [1] (as a grey band). Figure 24 shows good agreement between our result and the experimental values shown, as well as the experimental average.

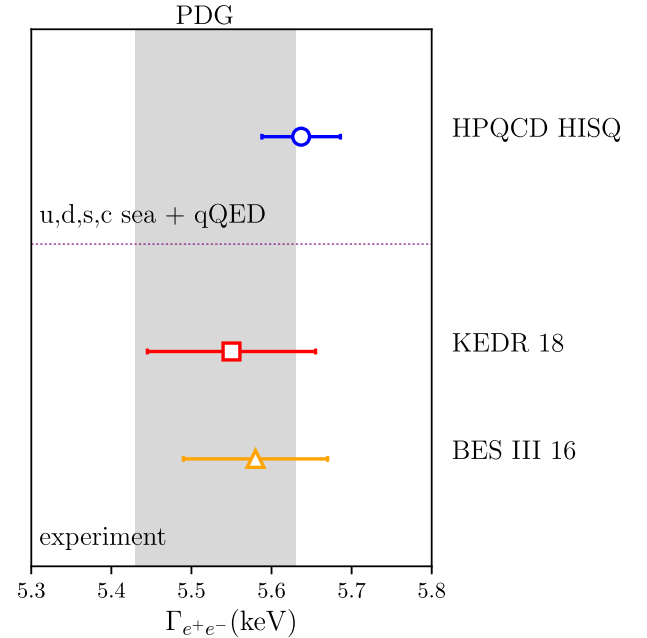


FIG. 24. A comparison of the width for J/ψ decay to e^+e^- implied by our new results for $f_{J/\psi}$ to that obtained from two recent experiments. The point labeled “KEDR 18” is from [54] and the point labeled “BES III 16” is from [55]. The grey bands are the $\pm 1\sigma$ bands from the Particle Data Group average [1].

The lattice QCD result is now more accurate than the experimental values.

VI. VECTOR CORRELATOR MOMENTS AND a_μ^c

With new results expected from the Fermilab $g-2$ experiment soon there has been a concerted effort by the lattice community to understand and control systematic effects in the lattice QCD calculation of the HVP contribution to the anomalous magnetic moment of the muon. Since the most accurate values for the HVP currently come from experimental results on $R(e^+e^- \rightarrow \text{hadrons})$, it is also important to compare lattice QCD results to these, disaggregated by flavor where possible.

The first calculation of the quark-line connected c -quark contribution to the HVP, a_μ^c , was given in [66] using results for the time moments of vector charmonium current-current correlators calculated in [31]. The time moments are defined by

$$G_n = Z_V^2 \sum_t t^n C_V(t), \quad (33)$$

where $C_V(t)$ is the vector current-current correlator and Z_V is the vector current renormalization factor, discussed in Sec. V. Note that $t \in \{-L/2 + 1, -L/2 + 2, \dots, L/2\}$.

The even-in- n time moments for $n \geq 4$ can be related to the derivatives at $q^2 = 0$ of the renormalized vacuum polarization function [67], $\hat{\Pi}(q^2) \equiv \Pi(q^2) - \Pi(0)$, by

$$G_n = (-1)^{n/2} \frac{\partial^n}{\partial q^n} q^2 \hat{\Pi}(q^2) \Big|_{q^2=0}. \quad (34)$$

This means that $\hat{\Pi}(q^2)$ can be reconstructed, using Padé approximants, from the G_n [66] and fed into the integral over q^2 that yields the quark-line connected HVP contribution to a_μ [68]. Only time moments of low moment number are needed to give an accurate result for a_μ^c because the integrand is dominated by small q^2 . We will give results for the four lowest moments, $n = 4, 6, 8, 10$, improving on the values given in [31]. The improvement comes mainly through the use of a more accurate vector current renormalization as well as an improved method for reducing lattice spacing uncertainties but we also use second-generation gluon field configurations that include c quarks in the sea and calculate, rather than estimate, the impact of the leading QED effects.

$\hat{\Pi}(q^2)$ and hence a_μ^c can also be determined from experimental results for $R_c \equiv R(e^+e^- \rightarrow c\bar{c} \rightarrow \text{hadrons})$ as a function of squared center-of-mass energy, s . This can be done using inverse- s moments

$$\mathcal{M}_k \equiv \int \frac{ds}{s^{k+1}} R_c(s). \quad (35)$$

R_c is obtained from the full e^+e^- rate from just below the c threshold upwards by subtracting the background contribution from u, d , and s quarks perturbatively, see e.g., [63].

The relationship between G_{2k+2} and \mathcal{M}_k is then

$$G_{2k+2} = \frac{(2k+2)! \mathcal{M}_k}{12\pi^2 Q^2}. \quad (36)$$

A comparison of our correlator time moments calculated on the lattice and extrapolated to the continuum limit to the inverse- s moments determined from experiment is equivalent to a test of the agreement of the results for a_μ^c in the two cases.

A. Vector correlator moments: Pure QCD and QCD+QED results

Table XII gives our raw results for the time moments of the same vector current-current correlators from which we have determined the mass and decay constant of the J/ψ meson in Secs. III and V. Notice that the statistical uncertainties are tiny. The correlators make use of a local vector current that must be renormalized as discussed in Sec. V. The results in Table XII are calculated *before* renormalization and are given in lattice units. The quantity that is tabulated is

$$\left(\frac{G_n}{Z_V^2} \right)^{1/(n-2)}. \quad (37)$$

We take the $(n-2)$ th root to reduce all results to the same dimensions [31]. To normalize the time moments we use the Z_V values at $\mu = 2$ GeV given in Table X that were used for $f_{J/\psi}$ in Sec. V.

Table XII also gives the result of including quenched QED as the ratios R_{QED}^0 for each rooted moment (at fixed am_c). These values are all very slightly less than 1, by up to 0.1% for $n = 4$, and 0.2% for $n = 10$. We can also test the finite-volume dependence of the quenched QED effect using sets 5, 7 and 8 and the results are shown in Fig. 25. There is no visible volume dependence in the QED effect on time moments at the level of our statistical uncertainties. This is to be expected, as seen for the J/ψ mass and decay constant in Secs. III and V, since the vector current being used here is electrically neutral.

To fit the results as a function of lattice spacing it is convenient to work with the dimensionless combination:

$$M_{J/\psi}(G_n)^{1/(n-2)}, \quad (38)$$

using our $M_{J/\psi}$ masses from Table III. The removal of dimensions reduces the uncertainty coming from the value of the lattice spacing. At the same time this quantity also has reduced sensitivity to mistuning of the valence c -quark mass because the m_c dependence is largely canceled by $M_{J/\psi}$. We fit the quantity defined in Eq. (38) as a function

TABLE XII. Time moments of charmonium vector current-current correlators calculated on the ensembles in Table I. The results tabulated are values of $(G_n/Z_V^2)^{1/(n-2)}$ in lattice units along with their statistical uncertainties, given for $n = 4, 6, 8$ and 10 in columns 2, 3, 4 and 5. Uncertainties are statistical only. Note that the results for different moments are correlated because they are determined from the same correlation functions. The results marked with a * and † are for deliberately mistuned am_c values as detailed in the caption to Table III. Also included are the ratios at fixed am_c , denoted R_{QED}^0 , of QCD + QED to QCD results for each rooted moment on a subset of ensembles.

| Set | $n = 4$ | $n = 6$ | $n = 8$ | $n = 10$ | $R_{\text{QED}}^0[n = 4]$ | $R_{\text{QED}}^0[n = 6]$ | $R_{\text{QED}}^0[n = 8]$ | $R_{\text{QED}}^0[n = 10]$ |
|-----|---------------|---------------|--------------|--------------|---------------------------|---------------------------|---------------------------|----------------------------|
| 1 | 0.389670(40) | 0.949791(62) | 1.410524(75) | 1.815497(88) | ... | ... | ... | ... |
| 2 | 0.396283(22) | 0.961260(35) | 1.425498(42) | 1.833868(49) | 0.999954(26) | 0.999910(17) | 0.999858(15) | 0.999810(15) |
| 3 | 0.400779(15) | 0.969045(24) | 1.435671(28) | 1.846369(33) | ... | ... | ... | ... |
| 4 | 0.511194(12) | 1.164351(19) | 1.701040(26) | 2.184698(34) | ... | ... | ... | ... |
| 6 | 0.5206344(85) | 1.181180(14) | 1.724311(19) | 2.214708(24) | 0.9998455(15) | 0.9997169(11) | 0.9995987(10) | 0.9994908(11) |
| 6* | 0.5254224(87) | 1.189687(14) | 1.736041(19) | 2.229780(25) | ... | ... | ... | ... |
| 8 | 0.5254560(47) | 1.1897785(76) | 1.736217(10) | 2.230069(13) | ... | ... | ... | ... |
| 9 | 0.70981(13) | 1.53941(21) | 2.24688(27) | 2.90799(32) | ... | ... | ... | ... |
| 10 | 0.723760(11) | 1.566115(20) | 2.285959(27) | 2.959283(36) | 0.999554(24) | 0.999312(20) | 0.999124(20) | 0.998995(22) |
| 11 | 0.731489(11) | 1.580936(18) | 2.307649(25) | 2.987715(32) | ... | ... | ... | ... |
| 12 | 1.070736(33) | 2.276543(58) | 3.355470(80) | 4.37418(10) | 0.999096(59) | 0.998767(49) | 0.998584(48) | 0.998489(48) |
| 13 | 1.114660(44) | 2.366266(78) | 3.48827(11) | 4.54699(14) | ... | ... | ... | ... |
| 14 | 1.431378(91) | 3.03675(16) | 4.49434(22) | 5.86769(29) | ... | ... | ... | ... |
| 14† | 1.46556(17) | 3.10710(31) | 4.59734(43) | 6.00058(56) | ... | ... | ... | ... |
| 15 | 1.91475(23) | 4.06357(42) | 6.02429(55) | 7.86806(66) | ... | ... | ... | ... |

of lattice spacing, allowing for quark-mass mistuning effects of both valence and sea quarks to derive results in the physical continuum limit. We do this as before using the fit function given in Eq. (5). Values in the physical continuum limit are then divided by $M_{J/\psi}$ from experiment to obtain our final results for $G_n^{1/(n-2)}$ in GeV^{-1} . In doing this we allow an uncertainty of 0.7 MeV in $M_{J/\psi}$ from

annihilation to a photon (see Sec. III) since this effect is not included in our results.

Figure 26 plots the results for the rooted moments multiplied by $M_{J/\psi}$ as a function of $(am_c)^2$. Also shown is the fit result from Eq. (5). Only the pure QCD lattice results are shown for clarity; those including the effect of quenched QED are very close to them. The fit result plotted is that for the QCD + QED case.

Table XIII gives our QCD + QED results for the 4th, 6th, 8th and 10th rooted moments in the physical continuum limit. These are obtained from a simultaneous fit to all of the moments, including the correlations between them (since they are derived from the same correlators). The fit has a $\chi^2/\text{d.o.f.}$ of 0.62 for an singular value decomposition (svd) cut of 1×10^{-3} .

Column 3 of Table XIII gives the results derived from experimental data for $R(e^+e^- \rightarrow \text{hadrons})$ and $\Gamma_{\ell\ell}$ and mass for the J/ψ and ψ' by [69] for comparison (see Sec. VI). We have converted these results into the quantity that we calculate according to Eq. (36). We see agreement within 2σ for $n \geq 6$ with the values derived from experiment, but a 2.4σ tension at $n = 4$. The results given from [69] correspond to their standard selection of experimental datasets. Results shift by $\pm 1\sigma$ for other selections. Note that the lattice QCD results are now much more precise than those determined from experiment. The comparison between lattice QCD and experiment will be discussed further in Sec. VI B.

Column 4 of Table XIII gives the final impact of quenched QED, including the quark mass retuning, on

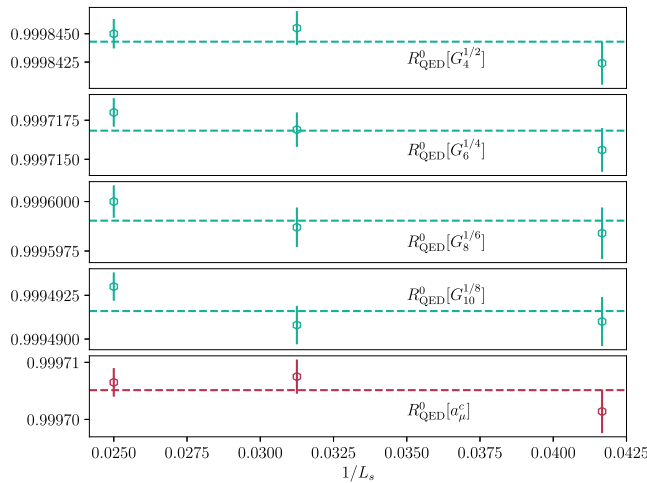


FIG. 25. A study of the volume dependence of the electromagnetic correction to the first four time moments of the vector current-current correlator and to a_μ^c on sets 5–7. There is no observable dependence on the lattice spatial extent, L_s , as can be judged by comparison to the dashed horizontal lines at the weighted averages of the points.

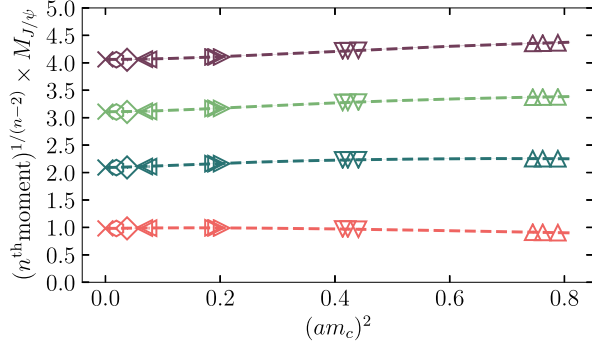


FIG. 26. The four lowest time moments and their extrapolation to $a = 0$. The symbols give results for the rooted moment multiplied by $M_{J/\psi}$ with different symbols denoting different groups of ensembles with similar lattice spacing. The different colors pick out the different moments, from $n = 4$ at the bottom to $n = 10$ at the top of the plot. Only the results from the pure QCD calculation at well-tuned c -quark masses are shown for clarity. Uncertainties are too small to be visible. The extrapolation for all the moments are performed simultaneously including correlations between moments determined from the same current-current correlators. The dashed lines give the QCD + QED fit curve using Eq. (5) and the colored crosses mark the result in the continuum limit at physical quark masses.

the moments. We see that the ratios, $R_{\text{QED}}[G_n^{1/(n-2)}]$, are greater than 1, in contrast to the R_{QED}^0 of Table XII that are less than 1. As discussed in Sec. II B, the inclusion of QED means that the c -quark mass must be retuned downwards. The rooted time moments are approximately inversely proportional to the quark mass and so they increase under this retuning, more than offsetting the direct effect of QED seen in R_{QED}^0 .

Table XIV gives the error budget for the G_n . The total uncertainty in all cases is below 0.2%.

B. Discussion: Vector correlator moments

Our new results for the time moments of vector current-current correlators improve significantly on earlier lattice

TABLE XIII. QCD + QED results in the physical continuum limit for the first four time moments (column 2) compared with the results extracted from experiment in column 3 [69]. Agreement within 2σ is seen for all except the 4th moment, but the lattice QCD results are much more accurate. Column 4 gives the effect of quenched QED as a ratio of the physical results in QCD + QED to those in pure QCD.

| n | $G_n^{1/(n-2)}$ GeV $^{-1}$ | $(G_n^{\text{exp}})^{1/(n-2)}$ GeV $^{-1}$ | $R_{\text{QED}}[G_n^{1/(n-2)}] \dots$ |
|-----|-----------------------------|--|---------------------------------------|
| 4 | 0.31715(49) | 0.3110(26) | 1.00106(13) |
| 6 | 0.67547(84) | 0.6705(31) | 1.00069(11) |
| 8 | 1.0041(11) | 0.9996(36) | 1.00047(10) |
| 10 | 1.3117(13) | 1.3080(37) | 1.00037(10) |

TABLE XIV. Error budget for $G_n^{1/(n-2)}$ as a percentage of the final answer.

| | $G_4^{1/2}$ | $G_6^{1/4}$ | $G_8^{1/6}$ | $G_{10}^{1/8}$ |
|---------------------|-------------|-------------|-------------|----------------|
| $a^2 \rightarrow 0$ | 0.06 | 0.05 | 0.04 | 0.03 |
| Z_V | 0.04 | 0.02 | 0.02 | 0.02 |
| Pure QCD Statistics | 0.03 | 0.02 | 0.02 | 0.02 |
| QCD+QED Statistics | 0.01 | 0.01 | 0.01 | 0.01 |
| Sea mistunings | 0.06 | 0.03 | 0.03 | 0.03 |
| Valence mistunings | 0.01 | 0.00 | 0.00 | 0.00 |
| $M_{J/\psi}$ | 0.02 | 0.02 | 0.02 | 0.02 |
| w_0 | 0.10 | 0.08 | 0.06 | 0.05 |
| w_0/a | 0.06 | 0.05 | 0.05 | 0.04 |
| Total | 0.15 | 0.12 | 0.11 | 0.10 |

QCD calculations and are now more accurate than results derived from experiment.

Figure 27 compares our new results for the 4th and 6th moments to earlier lattice QCD results. Comparison for the 8th and 10th moments gives a very similar picture and so is not shown. The first lattice QCD calculation of the time moments of vector charmonium current-current correlators was given by HPQCD in [31] using HISQ valence quarks on $n_f = 2 + 1$ asqtad gluon field configurations. Our new results have an uncertainty almost ten times smaller than these. The error budget in the earlier results was dominated by the uncertainty in Z_V from the use of continuum perturbation theory in the matching factors and there was also a sizeable uncertainty from the lattice spacing. These uncertainties have been enormously reduced here and in addition we no longer need an uncertainty from missing QED effects. We also show a comparison with the subsequent results from the JLQCD Collaboration [70] using domain-wall quarks on $n_f = 2 + 1$ gluon field configurations. JLQCD does not give a value for the 4th moment because of discretization effects in their formalism [tree level $\mathcal{O}(a^2)$]. The dominant uncertainties in their results are from statistics and from the value of $t_0^{1/2}$ used to fix the lattice spacing, on which they have a 2% uncertainty. Good agreement is seen for all of the lattice QCD results.

Two of the most recent results from phenomenological determinations of the moments [63,69] are also compared in Fig. 27. The results from [69] include experimental datasets for the inclusive cross section that are both older and newer than those used in [63]. Results from [69]’s “standard” selection of datasets were given in Table XIII and are shown in Fig. 27 in red. We also show, in orange, the results from the maximal set (all experimental information available at that point) and the minimal set (datasets that are needed to cover the full \sqrt{s} range from 2 GeV to 10.5 GeV without gaps, keeping the most accurate results). Note that the resonance parameters are the same for all selections. We see that the variation with dataset selection covers almost 1σ for the 4th moment, but much less for the

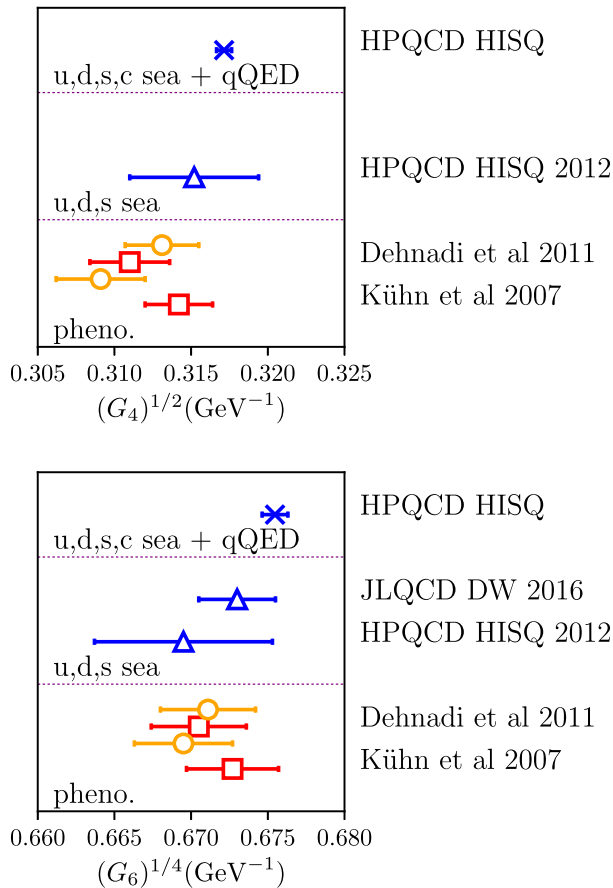


FIG. 27. Comparison of our new result to those of previous lattice QCD calculations for the 4th and 6th time moments (appropriately rooted) of the charmonium vector current-current correlator. Our new result obtained here on $n_f = 2 + 1 + 1$ gluon field configurations and including the effect of quenched QED is given at the top (blue cross). HPQCD’s 2012 result on $n_f = 2 + 1$ gluon field configurations with HISQ valence c quarks is marked “HPQCD HISQ 2012” [31]. JLQCD’s 2016 result using $n_f = 2 + 1$ domain-wall quarks is marked “JLQCD DW 2016” for the 6th moment only. We also compare to results (open red squares) denoted “pheno.” that are derived from experimental data for the cross section for e^+e^- to hadrons as a function of center-of-mass energy, by determining the $c\bar{c}$ component. The points plotted come from [63,69]. Open orange circles show alternative selections of datasets from [69]; the upper value is for the “maximal” set and the lower value for the “minimal” set.

6th moment. This is also reflected in the differences between [63,69].

These phenomenological analyses must subtract the “noncharm” background from experimental results for $R(e^+e^- \rightarrow \text{hadrons})$ to leave R_c for Eq. (35). R_c is defined to be the result from diagrams with a charm quark loop connected to a photon at both ends [63] i.e., the quark-line connected vector current-current correlator that we study on the lattice. The subtracted background includes QED effects for the noncharm and singlet (quark-line disconnected) contributions. The remainder R_c then includes the

QED effects associated with the $c\bar{c}$ loop. The dominant source of uncertainty in R_c comes from the charmonium resonance (J/ψ and ψ') region and is set by the uncertainty in Γ_{ee} for these states. The fractional uncertainty is approximately the same for all moments [63,69]. When the $(n-2)$ th root is taken the fractional uncertainty then falls with increasing n .

Good agreement is seen between the phenomenological results and our new lattice results for $n = 6, 8$ and 10 , although the lattice results are systematically at the upper end of the phenomenological range. The largest discrepancy is a 2.8σ tension for the 4th moment between us and the results of [69] for their minimal selection of datasets. The tension is 2.4σ for the standard selection, and below 2σ for the maximal selection and for the results of [63]. The σ here is that for the phenomenological results since the lattice uncertainty is much smaller. Because the 4th moment dominates the determination of a_μ^c , this tension between lattice QCD + QED and some of the phenomenological results carries over to a_μ^c , to be discussed in the next section.

The time moments can also be used to determine a value for \bar{m}_c by comparing to $\mathcal{O}(\alpha_s^3)$ continuum QCD perturbation theory and this was the focus of [63,69]. We do not do this here because the scale of α_s is rather low in these determinations meaning that uncertainties from missing higher-order corrections can be substantial. We prefer instead the method of [26], which enables a higher scale to be used in the perturbation theory. We have checked, however that the m_c value that would be obtained from the time moments is consistent with both [26] and the value given in Sec. IV.

C. a_μ^c : Pure QCD and QCD + QED results

To calculate the quark-line connected HVP contribution to a_μ from c quarks, a_μ^c , we can either use the physical results for the vector current-current correlator time moments discussed in the previous subsection or we can calculate a_μ^c on each lattice ensemble and perform a fit as a function of lattice spacing to extrapolate directly to the continuum limit. We will do the latter here.

The values of a_μ^c on each lattice are given in Table XV. These are determined from the time moments rescaled by the J/ψ mass on each lattice:

$$\frac{M_{J/\psi} G_n^{1/(n-2)}}{M_{J/\psi}^{\text{expt}}}. \quad (39)$$

As discussed in Sec. VIA rescaling by $M_{J/\psi}$ reduces the lattice spacing uncertainty and the impact of mistuning the c -quark mass. This was used for lighter quark masses in [71] (see also [72]). The reduced effect of mistuning is clear from comparing the mistuned results in Table XV to those in Table XII.

Table XV also includes results on the two ensembles, sets 3A and 3B, that allow direct comparison of the effects of

TABLE XV. Values of a_μ^c on the ensembles of Table I and the direct quenched QED correction on a subset of those ensembles. Those marked with a * and † are at deliberately mistuned c masses (see caption to Table III). The uncertainties quoted are correlated through the value of $M_{J/\psi}$ (for all ensembles, see text) and Z_V (for ensembles at a given β).

| Set | $a_\mu^c \times 10^9$ | $R_{\text{QED}}^0[a_\mu^c]$ |
|-----|-----------------------|-----------------------------|
| 1 | 1.23183(78) | ... |
| 2 | 1.24522(75) | 1.000478(80) |
| 3 | 1.25431(77) | ... |
| 3A | 1.25518(49) | ... |
| 3B | 1.25485(48) | ... |
| 4 | 1.40782(91) | ... |
| 6 | 1.41738(91) | 1.001080(89) |
| 6* | 1.42370(91) | ... |
| 8 | 1.42234(91) | ... |
| 9 | 1.47866(97) | ... |
| 10 | 1.48514(75) | 1.001416(83) |
| 11 | 1.48853(75) | ... |
| 12 | 1.4725(13) | 1.00141(15) |
| 13 | 1.4805(13) | ... |
| 14 | 1.4610(33) | ... |
| 14† | 1.4702(33) | ... |
| 15 | 1.4572(10) | ... |

strong-isospin breaking the sea. The ratio of the two results is 0.99974(14), so the results agree to within 0.03% (and 2σ), consistent with these effects being negligible here (see Sec. IID).

Table XV also gives the direct effect of quenched QED through the ratio $R_{\text{QED}}^0[a_\mu^c]$. Because the rescaled moments have less sensitivity to the c -quark mass these numbers are larger than 1 (unlike the results in Table XII) and reflect more closely the final impact of QED on a_μ^c . We observe no finite-volume dependence for the quenched QED corrections to a_μ^c , as for the correlator time moments. This is shown in Fig. 25.

The results from Table XV are shown in Fig. 28 along with our standard fit of the form given in Eq. (5). The fit has a $\chi^2/\text{d.o.f.}$ of 0.44. This fit obtains the physical values

$$\begin{aligned} a_\mu^c &= 14.606(47) \times 10^{-10}, & \text{QCD} \\ a_\mu^c &= 14.638(47) \times 10^{-10}, & \text{QCD + QED} \end{aligned} \quad (40)$$

along with $R_{\text{QED}}[a_\mu^c] = 1.00214(19)$. These results agree well (within 1σ) with those obtained using the extrapolated values for the moments from Table XIII and calculating a_μ^c in the continuum, as is seen in Fig. 28.

The error budget for our final value of a_μ^c is given in Table XVI. The largest uncertainties come from the determination of the lattice spacing, although this uncertainty is much reduced by our rescaling with $M_{J/\psi}$.

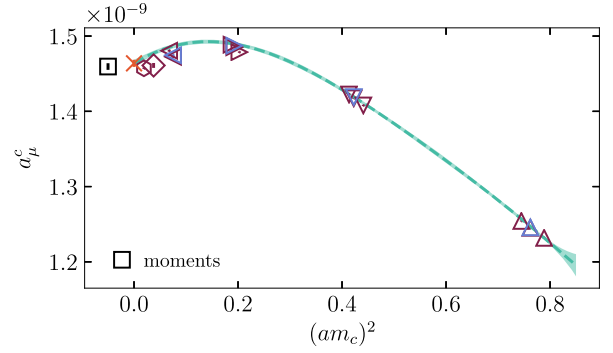


FIG. 28. Extrapolation to the continuum physical point of the connected charm HVP contribution to the anomalous magnetic moment of the muon. Different symbols denote results on groups of ensembles with similar lattice spacing. Results at deliberately mistuned c -quark masses are not plotted but are included in the fit. The red points correspond to pure QCD, the light blue points to QCD + QED and the dashed green fit curve plotted is that for QCD + QED. The continuum result (red cross) is compared to the result (open black square) obtained by calculating a_μ^c from the individually extrapolated time moments in Sec. VIA.

D. Discussion: a_μ^c

Our new result for the pure QCD case [Eq. (40)] is compared to earlier lattice QCD results with realistic sea quark content in Fig. 29. Our new result (the top point on the plot) is much more accurate than the earlier results. With respect to the first calculation of a_μ^c that also used HISQ quarks [26] we have greatly reduced the previous dominant sources of uncertainty from Z_V and the determination of the lattice spacing.

With respect to results using other formalisms, we give one figure to demonstrate the control of discretization effects that is possible with the HISQ formalism. Figure 30 compares the approach to the continuum limit of our results (from Table XV) with results from BMWc [74], for which the continuum extrapolated result is shown in Fig. 29. The points plotted from [74] are estimates of the positions read from Fig. S4 of that reference, and do not include any

TABLE XVI. Error budget for a_μ^c from our fit to a_μ^c values on each ensemble.

| | a_μ^c |
|---------------------------|-----------|
| $a^2 \rightarrow 0$ | 0.15 |
| Z_V | 0.07 |
| Pure QCD Statistics | 0.08 |
| QCD + QED Statistics | 0.01 |
| w_0/a | 0.16 |
| w_0 | 0.18 |
| Sea mistunings | 0.09 |
| Valence mistunings | 0.03 |
| $M_{J/\psi}^{\text{exp}}$ | 0.05 |
| Total | 0.32 |

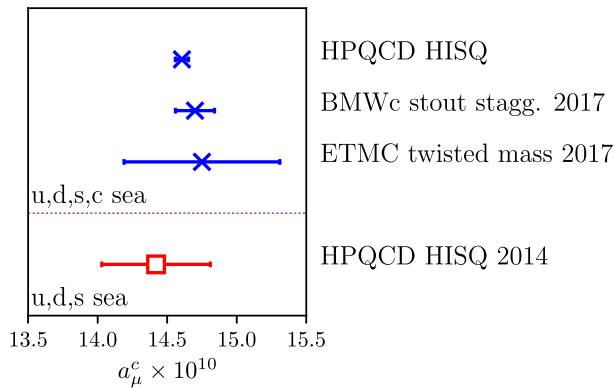


FIG. 29. Comparison of lattice QCD results (not including QED) for the connected c quark HVP contribution to a_μ , a_μ^c . Results are divided according to the number of sea quark flavors included in the gluon field configurations on which the calculation was done. The first result, labeled “HPQCD HISQ 2014” is from [26] using values of time moments determined in [31] using HISQ valence quarks on gluon field configurations including $n_f = 2 + 1$ flavors of asqtad sea quarks. The other results all include $n_f = 2 + 1 + 1$ flavors of sea quarks. The result labeled “ETMC twisted mass 2017” uses the twisted mass formalism [73] and that labeled “BMW stout stagg. 2017” a smeared staggered quark action [74]. Our new result [from Eq. (40)] labeled “HPQCD HISQ” agrees with, but is much more accurate than, these earlier results.

indication of statistical uncertainties. The BMWc stout staggered quark action has $\mathcal{O}(a^2)$ discretization errors at tree level since it uses an unimproved derivative in its version of the Dirac equation. Figure 30 shows that the price to be paid for not improving the discretization is a very large discretization effect. This is particularly evident when working with heavier quarks such as charm, since it means that the dominant $(\Lambda a)^2$ effects have $\Lambda \approx 1$ GeV, as here. This means, for example, that the BMWc points at finest lattice spacing (~ 0.06 fm) are about as far (20% away) from the continuum limit as our points at our coarsest lattice spacing (~ 0.15 fm). Our results at $a \sim 0.06$ fm are within 1% of the continuum limit, allowing us to achieve a sub-1% uncertainty in the final value.

We find that the impact of quenched QED on the result for a_μ^c is $+0.214(19)\%$ [Eq. (40)]. This is a shift in a_μ^c in the presence of the dominant QED effect of

$$\delta a_\mu^c = +0.0313(28) \times 10^{-10}. \quad (41)$$

We can compare this to the result obtained by ETMC in [5] following work on the QED effect on the renormalization of quark bilinears in [24]. The ETMC value is $+0.0182(36) \times 10^{-10}$, 2.8σ smaller than ours.

The two calculations of the quenched QED effect are different. Ours is a direct calculation of the quenched QED effect, retuning the valence quark mass through determination of a meson mass in the usual way. The ETMC

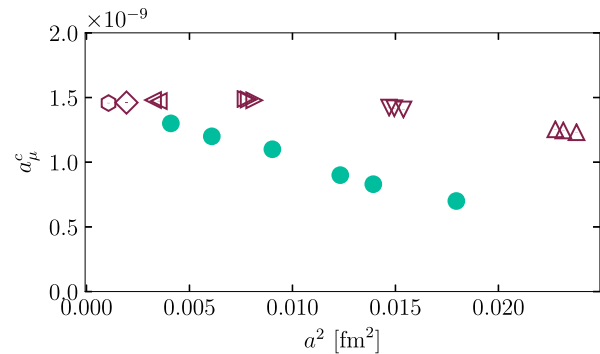


FIG. 30. Comparison of the discretization effects in a_μ^c in our results from Table XV (red open symbols) and those from the BMW Collaboration in [74] (filled blue circles) that use a less highly improved staggered quark action. The filled blue circles only give estimates of the position of the BMW data points and do not indicate the statistical uncertainties which are much smaller than the size of the points.

calculation is perturbative in quenched QED and fixes the valence quark masses so that they agree in the $\overline{\text{MS}}$ scheme at 2 GeV in QCD + QED and pure QCD. It is likely that it is this difference in scheme for defining how QCD and QCD + QED are compared that is responsible for the tension between the two values. Our results in Sec. IV show that the quark mass in the $\overline{\text{MS}}$ scheme is lower in QCD + QED than in QCD (at scales above \bar{m}_c) when the quark mass is tuned so that $M_{J/\psi}$ agrees with experiment in the two cases. This leads us to expect a larger result for the impact of quenched QED on a_μ^c with our tuning. Once full lattice QCD + QED calculations are underway tuning of the quark masses will be done through matching of meson masses to experiment.

Figure 31 includes a comparison of our result for a_μ^c , now in QCD + QED, with values obtained using the moments determined from J/ψ and ψ' properties and the inclusive cross section for $e^+e^- \rightarrow \text{hadrons}$, removing contributions from quarks other than c . The results for these moments from [63,69] were discussed and compared to our results in Sec. VI B. In Fig. 31 we have converted the moments into a result for a_μ^c for comparison. As with the moments, we see a 2.5σ tension with the [69] result using the standard selection of datasets [$a_\mu^c = 14.03(24) \times 10^{-10}$], and a larger tension with the minimal selection of datasets. There is agreement within 2σ for the maximal selection of datasets from [69] and with [63]. Our result may then provide a pointer to the selection of $R_{e^+e^-}$ datasets for the phenomenological determination and/or indicate an issue with the perturbation theory used to subtract the $u/d/s$ contribution to obtain $R_c(s)$.

More recent determinations of the complete HVP contribution to a_μ using results from $R_{e^+e^-}$ are given in [53,75]. Although the c component is not separated out, the contribution from the J/ψ resonance is given as $6.26(19) \times 10^{-10}$ by [53] and $6.20(11) \times 10^{-10}$ by [75]. We can also

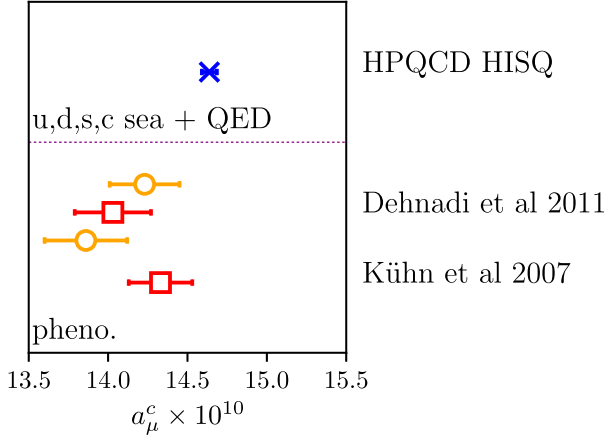


FIG. 31. Comparison of our lattice QCD + QED result (blue cross) for the connected c quark HVP contribution to a_μ , a_μ^c , with results determined from experimental information. The red open squares, denoted “pheno.,” use the charmonium moments from $R_{e^+e^-}$ given in [63,69] to determine a_μ^c . The orange open circles give the alternative maximal (upper) and minimal (lower) inclusive cross-section datasets from [69].

readily determine the contribution to a_μ^c from the J/ψ resonance alone since in that case [76]

$$G_n = n! \frac{f_{J/\psi}^2}{M_{J/\psi}^n}. \quad (42)$$

Using our value for $f_{J/\psi}$ from Eq. (29) and the experimental value for $M_{J/\psi}$ [1] gives

$$a_\mu^c(J/\psi) = 6.345(53) \times 10^{-10}. \quad (43)$$

This is in good agreement with the results determined above from the experimental J/ψ parameters, but more accurate, reflecting the fact that our result for $\Gamma_{e^+e^-}$ in Fig. 24 agrees with experiment but has smaller uncertainty.

The J/ψ contribution provides almost half of a_μ^c —we conclude that it is the rest of the contribution, from the inclusive cross section above the resonance region, that causes the tension between our results for a_μ^c and that from $R_{e^+e^-}$ for some selections of experimental datasets. The tension then amounts to 7(3)% of this nonresonant cross section.

VII. CONCLUSIONS

We have performed the first $n_f = 2 + 1 + 1$ lattice QCD computations of the properties of ground-state charmonium mesons. These have been done using the HISQ action to calculate quark-line connected two-point correlation functions on gluon field configurations that include u/d quark masses going down to the physical point. The small discretization effects in the HISQ action and high statistics achievable have given us good control over both the

continuum and chiral extrapolations and have enabled us to obtain smaller uncertainties than previous lattice QCD computations of these properties (including previous calculations by HPQCD). At the same time we have improved the tuning of the bare c -quark mass to update the value of \bar{m}_c . From the same correlators that we use for the masses and decay constants we have also derived an improved result for the c quark HVP contribution to the anomalous magnetic moment of the muon.

The precision possible for c quark correlators with the HISQ action makes it possible to determine the impact of the c quark’s electric charge. We do this directly and nonperturbatively in quenched QED by multiplying an appropriate U(1) field into our gluon field configurations. We tune the bare c -quark mass so that the J/ψ mass agrees with experiment in both QCD + QED and QCD and we calculate mass and vector renormalization constants in the RI-SMOM scheme in both cases, performing a full analysis as a function of μ to determine the c -quark mass in the $\overline{\text{MS}}$ scheme.

Here we collect our final QCD + QED results [from Eqs. (10), (17), (29), (30), (40)] before discussing each in turn:

$$\begin{aligned} M_{J/\psi} - M_{\eta_c} &= 0.1203(11) \text{ GeV} \\ \bar{m}_c(3 \text{ GeV}) &= 0.9841(51) \text{ GeV} \\ f_{J/\psi} &= 0.4104(17) \text{ GeV} \\ f_{\eta_c} &= 0.3981(10) \text{ GeV} \\ a_\mu^c &= 14.638(47) \times 10^{-10}. \end{aligned} \quad (44)$$

Error budgets are given in Tables V, VII, XI and XVI respectively. Our error budgets do not include an error for missing QED effects for sea quarks or from having $m_u = m_d$ in the sea. We expect the former to dominate (see Sections II C and II D) and estimate this at 10% of the size of the valence quark QED effects. This is then a negligible error in every case.

The precision of our result for the charmonium hyperfine splitting allows us to resolve, for the first time, the sign and magnitude of the anticipated difference between the lattice and experimental results arising from the fact that we do not include quark-line disconnected correlation functions. We take this difference to be the effect of the η_c decay to two gluons which is prohibited in the lattice calculation, and conclude that $\Delta M_{\eta_c}^{\text{annihln}} = +7.3(1.2) \text{ MeV}$.

The effect of QED on the hyperfine splitting is fairly substantial (1.4%) and the largest effect that we observe here. This has 3 components that all act in the same direction: a direct effect of 0.7%, 0.1% from retuning the c -quark mass and 0.6% from J/ψ annihilation to a photon that we add by hand.

Our updated value of the charm quark mass (in the $\overline{\text{MS}}$ scheme at a scale of 3 GeV) includes the effect of QED on

the bare c quark mass, tuned so that $M_{J/\psi}$ matches experiment, and on the mass renormalization constant Z_m determined on the lattice using the intermediate RI-SMOM scheme. The addition of results at a finer lattice spacing has improved the uncertainty slightly over HPQCD's earlier result [46].

The impact of QED on \bar{m}_c is small since QED effects tend to cancel between the retuning needed and changes in Z_m . At a scale of 3 GeV we see a $-0.18(2)\%$ effect, falling towards zero at a scale of \bar{m}_c .

Our result for the J/ψ decay constant is the most precise to date and acts as a subpercent test of QCD. The gain in precision from the 2012 HPQCD calculation of [31] is a result of the use of a more accurate renormalization of the vector current [16] as well as gluon field configurations with a wider range of sea u/d quark masses and lattice spacing values. We can use our result for $f_{J/\psi}$ to determine a value for the width for J/ψ decay to a lepton-antilepton pair [repeating Eq. (32)]:

$$\Gamma(J/\psi \rightarrow e^+e^-) = 5.637(47)(13) \text{ keV}. \quad (45)$$

This is more accurate than the current average of experimental results [1].

The impact of quenched QED on $f_{J/\psi}$ is $+0.2\%$, since the retuning of the c -quark mass offsets some of the direct effect. The effect on f_{η_c} is almost the same so that the ratio of $f_{J/\psi}$ to f_{η_c} remains the same. This ratio is determined here to be $1.0289(19)$, so that it is definitely greater than 1; this was not completely clear from earlier calculations.

Our results for the time moments of the charmonium vector current-current correlators also provide a new level of accuracy for these quantities, improving by a factor of 10 over the first such calculations in [31]. Our results are given in Table XIII. We see some tension for the lowest (4th) moment with phenomenological results derived from $R(e^+e^- \rightarrow \text{hadrons})$ in [69] when particular selections of experimental datasets are made.

We use the time moments to derive the connected c quark HVP contribution to the anomalous magnetic moment of the muon, a_μ^c . Although this is not a large part of the total HVP contribution and so improving its uncertainty has little impact on the full HVP contribution, nevertheless it is a piece that can be calculated very accurately in lattice QCD and provides a test case for comparison of lattice calculations and a comparison with phenomenology.

Our result for a_μ^c improves the accuracy by a factor of 3 over earlier lattice QCD values [26,73,74]. Comparison of our result for a_μ^c to that determined from phenomenology can be divided into contributions from narrow resonances and from the continuum $e^+e^- \rightarrow c\bar{c}$. The contribution from the J/ψ agrees well between our result and phenomenology, with our result being more accurate (see Sec. VID). This reflects the situation described above for $f_{J/\psi}$ and $\Gamma_{\ell\ell}$.

The total a_μ^c derived from the time moments determined from experimental data on $R(e^+e^- \rightarrow \text{hadrons})$ when the component from a $c\bar{c}$ loop is separated out shows some tension with our results, depending on which experimental datasets are used above the resonance region. Our central value is higher, tending to reduce by a small amount the discrepancy in a_μ between existing experiment and the Standard Model. We should stress, however, that more complete determinations of a_μ , for example in [53,75], do not separate out a_μ^c and so we cannot make a direct comparison to them.

We also determine the impact of quenched QED on a_μ^c in a scheme in which the c -quark mass is tuned from $M_{J/\psi}$ in both QCD + QED and pure QCD. We find [repeating Eq. (41)]

$$\delta a_\mu^c = +0.0313(28) \times 10^{-10}. \quad (46)$$

This is a 0.2% effect and dominated by the impact of retuning the c -quark mass.

Our result for a_μ^c has an accuracy of 0.3% . Sub- 0.5% uncertainty is the aim for lattice QCD calculations of the full HVP contribution to a_μ . We have shown that this is possible, for a small piece of the HVP, at least.

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APPENDIX: Z_V AND Z_m DETERMINATION ON THE FINEST LATTICES

We can use the results of [16] to check the consistency of the Z_V value on set 14 that we present here and to obtain a value on set 15. We do this by fitting the RI-SMOM results for the local vector current in Table III of [16] to the expected functional form. This form is based on a power series in α_s evaluated in the $\overline{\text{MS}}$ scheme at a scale of $1/a$, which is the perturbative lattice-to- $\overline{\text{MS}}$ renormalization factor, remembering that the SMOM to $\overline{\text{MS}}$ renormalization

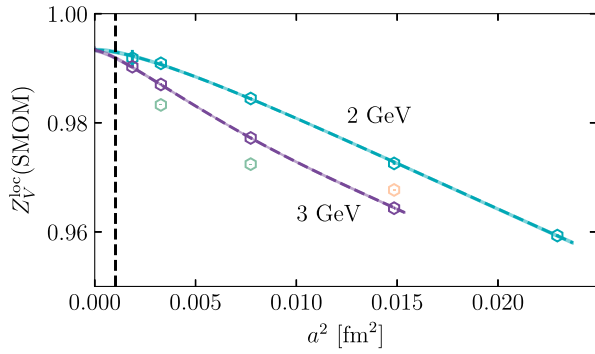


FIG. 32. Results for the local vector current renormalization factor in the RI-SMOM scheme compared to the fit form given in Eq. (A1). All of the data points shown are included in the fit but only the 2 and 3 GeV fit lines are drawn. The data points not on the fit lines correspond to $\mu = 2.5$ GeV (light orange) and 4 GeV (light green). The dashed line shows the value of a on the exafine lattices that allows us to determine a Z_V value there.

factor is exactly 1 in this case. In addition we must allow for possible discretization effects that depend on $a\mu$. The form we use is

$$Z_V^{\text{loc}}(\text{SMOM})(a, \mu) = 1 + \sum_{i,j=1}^{i=4, j=3} \left[c_i + d_{ij} \left(\frac{a\mu}{\pi} \right)^{2j} \right] \alpha_s^i. \quad (\text{A1})$$

This is very similar to the approach adopted in Appendix B of [77] using results for Z_V from the determination of form factors between two identical mesons at rest. As there, we fix the α_s coefficient to its known perturbative value of $-0.1164(3)$.

Figure 32 shows the Z_V data from [16] as hexagons, colored according to their μ value. The fit lines for 2 and 3 GeV are also shown. The fit has a $\chi^2/\text{d.o.f.}$ of 0.93. We note that the results from set 14 are included in this fit. The results from set 14, however, also agree with the fit result

TABLE XVII. Values of Z_m^{SMOM} obtained in the RI-SMOM scheme on set 14 in pure QCD. Results are given at two values of μ , listed in lattice units in column 1. They correspond approximately to 2 and 3 GeV. The correlation between the two numbers is 0.122.

| $a\mu$ | Z_m^{SMOM} |
|--------|---------------------|
| 0.4466 | 1.2925(39) |
| 0.6525 | 1.1785(11) |

when they are not included in the fit. As discussed in Sec. IV μ was slightly mistuned on set 14; the true values are 2.04 and 2.98 GeV rather than 2 and 3 GeV. At this small lattice spacing the variation in Z_V with μ (which is a discretization effect) is small enough that this small mistuning can be neglected.

Note that the underlying perturbation theory of Eq. (A1) should agree with that obtained from the fit in [77] and it does. The discretization effects are different in the two cases, of course. For RI-SMOM there is a momentum scale μ which we take as 2 GeV (although it can be taken as much smaller for Z_V [16]) and this sets the size of discretization effects as is clear from Fig. 32.

Using the fit of Eq. (A1) we may also extract Z_V values at finer lattice spacings where it may not be practical for us to perform direct calculations due to the computational cost of Landau gauge fixing. This includes the exafine lattices of set 15 in Table I with a lattice spacing adjusted for sea-mass mistuning of 0.032 fm. The value of Z_V from the fit for these lattices is 0.99296(21) at $\mu = 2$ GeV and 0.99186(18) at 3 GeV.

Results for the mass renormalization factor from the lattice to the RI-SMOM scheme, $Z_m^{\text{SMOM}}(\mu)$, determined on ultrafine set 14 are given in Table XVII at $\mu = 2$ and 3 GeV. These are calculated in the same way as that discussed in [46].

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