Improved nonrelativistic QCD for heavy-quark physics

G. Peter Lepage,* Lorenzo Magnea,† and Charles Nakhleh
Newman Laboratory of Nuclear Studies, Cornell University, Ithaca, New York 14853

Ulrika Magnea
State University of New York at Stony Brook, Stony Brook, New York 11794

Kent Hornbostel
The Ohio State University, Columbus, Ohio 43210
(Received 20 February 1992)

We construct an improved version of nonrelativistic QCD for use in lattice simulations of heavy-quark physics, with the goal of reducing systematic errors from all sources to below 10%. We develop power-counting rules to assess the importance of the various operators in the action and compute all leading-order corrections required by relativity and finite lattice spacing. We discuss radiative corrections to tree-level coupling constants, presenting a procedure that effectively resums the largest such corrections to all orders in perturbation theory. Finally, we comment on the size of nonperturbative contributions to the coupling constants.

PACS number(s): 12.38.Gc, 11.10.Gh, 12.38.Bx, 14.40.Gx

I. INTRODUCTION

Several papers in recent years have explored the possibility of substituting a nonrelativistic action for the usual Dirac action in lattice QCD simulations of heavy quarks [1–3]. In particular, this technique has been applied to simulations of the ψ and Υ families of mesons. Results from these simulations have been very encouraging. They not only capture the gross features of quarkonium physics but also are surprisingly accurate given the many approximations inherent in the simulations. Such success follows from a variety of properties unique to quarkonium states and from the algorithmic advantages of a nonrelativistic formulation of quark dynamics. This suggests the possibility of a truly reliable numerical study of quarkonium states using computing resources that are currently available, a study in which all systematic errors are identified, computed, and removed to some reasonable level of precision. In this paper we develop the outline for such a program and provide some of the ingredients needed to move from existing quarkonium studies to precision studies. Most of the techniques we describe are readily generalized for use in simulations of other bound states containing heavy quarks, such as D and B mesons.

The major tools for simulating gluon dynamics in QCD all involve Monte Carlo methods of one sort or another. Consequently, in simulating quarkonium states, we must worry about statistical as well as systematic errors. However, simulation data can be generated far more efficiently for quarkonium states than for ordinary hadrons, and thus the dominant errors for many of the most important quarkonium measurements are systematic. Here we focus only on these.

The nonrelativistic formulation of heavy-quark dynamics is referred to as nonrelativistic quantum chromodynamics (NRQCD). There are five potentially significant sources of systematic error when NRQCD is used to study quarkonium states.

(1) *Relativity.* The basic action for the heavy quarks incorporates the physics of the Schrödinger equation. Left out are relativistic corrections of $O(v^2)$, where v is the quark velocity. Since v^2 is approximately 0.3 for the ψ's and 0.1 for the Υ's, we expect errors of 10–30% due to relativistic corrections. Such errors can be systematically removed by adding new interactions to the heavy-quark action.

(2) *Finite lattice spacing.* As in all lattice simulations, there are errors resulting from the discretization of space and time. For our systems, such errors are $O(a^2p^2)$ and $O(aK)$, where a is the lattice spacing and p and K are the typical three-momentum and kinetic energy of a quark in the hadron. Since typically $a \sim 1/M$, where M is the quark mass, these errors are roughly the same order as those due to relativity. These may also be systematically removed by correcting the heavy-quark action.

(3) *Radiative corrections.* As in the Dirac action, the basic action in NRQCD contains only two parameters: the QCD coupling constant g, and the quark mass M.[1] However, each of the new interactions added to NRQCD

*Electronic address: gpl@lnssun1.tn.cornell.edu
†On leave from Università di Torino, Italy.

[1]Actually there is a third parameter E_0, which adjusts the origin of the nonrelativistic energy scale to coincide with that of the relativistic energy scale. However, this parameter affects only the absolute masses of hadrons and has no effect upon nonrelativistic quark dynamics, mass splittings, wave functions, etc. In principle E_0 may be computed, at least approximately, using perturbation theory.

to correct for relativity or finite lattice spacing introduces a new coupling constant. These new couplings can be treated as free parameters, to be adjusted by fitting to experimental data, but this significantly reduces the predictive power of a simulation. Alternatively one can try to compute these couplings in terms of g and M using perturbation theory, thereby reducing the number of parameters back to two. The radiative corrections to these coupling constants are determined by physics at distances of order the lattice spacing a, and therefore perturbation theory should be applicable provided a is small enough. However, a must not be too small. NRQCD is nonrenormalizable, and as a result the radiative corrections contain power-law ultraviolet divergences, such as g^2/aM, which make perturbation theory useless unless $a \sim 1/M$ or larger. Lattice spacings currently in use, where $g^2 \approx 1$, are probably suitable for both c and b quarks, and also seem small enough for perturbation theory to work. Radiative corrections of order 20–40 % could easily result, making these among the largest contributions at the order we are considering. We will see that they are well estimated using mean-field-theory techniques. Uncalculable corrections due to nonperturbative physics at short distances could be of order a few percent.

(4) *Finite lattice volume.* Quarkonium hadrons are much smaller than ordinary hadrons. Typical lattices in use today can easily be 10 Υ-radii across, making it unlikely that the finite volume of the lattice has much of an effect upon simulation results.

(5) *Light-quark vacuum polarization.* Hadrons built of heavy quarks are affected by light quarks through vacuum polarization. Such effects are usually very expensive to simulate numerically due to the inefficiency of the algorithms when quark masses are small. However, effects from light-quark vacuum polarization are likely to be small for quarkonium states. Some evidence comes from the decay widths of excited ψ and Υ mesons into D and B mesons, respectively. These decays result from light-quark vacuum polarization, and their widths are closely related to the energy shifts due to light quarks. The small size of these widths compared to typical mass splittings, together with model studies of this coupled-channel problem [4], suggests that light-quark vacuum polarization might affect quarkonium states at only the 10% level. Furthermore, the extrapolation from large to small light-quark masses should be quite smooth for low-lying quarkonium states since, unlike the ρ meson, for example, these are all effectively stable even for realistic light-quark masses.[2] Note finally that heavy-quark vacuum polarization has only a small effect upon quarkonium states since there is too little energy in such states to easily produce a heavy virtual quark and antiquark. For most purposes such effects can be ignored, though they are easily incorporated through perturbatively computed corrections to the gluon action.

This list suggests that we might be able to reduce systematic errors below 10% in quarkonium simulations using NRQCD. To achieve this goal we must compute all of the leading-order interactions that correct the action for relativity and finite lattice spacing as well as the leading radiative corrections for the most important of these interactions. Other sources of error are probably unimportant at this level, although including some light-quark vacuum polarization effects (by extrapolation) is both feasible and desirable. In this paper, we present all tree-level corrections to the NRQCD action that are relevant to work at this level of precision. Although we have only just started the analysis of radiative corrections, we also present here some general comments concerning the nature and treatment of these corrections.

Our analysis begins in Sec. II with the development of power-counting rules that allow us to determine the relative importance of various operators in the NRQCD action for analyses of quarkonium states. Such rules are trivial when one is considering light-heavy systems such as D or B mesons. They are more complicated for heavy-heavy systems since the heavy quark is not a spectator in such a hadron; in particular, the quark mass strongly affects the hadron's size and internal dynamics. In Sec. III, we compute the $O(v^2)$ corrections to the NRQCD action in the continuum for both Minkowskian and Euclidean space. In Sec. IV, we discretize the corrected NRQCD action, further modifying it to remove the leading errors due to the finite lattice spacing. In Sec. V, we discuss some general properties of the radiative corrections, we give estimates for the largest of these, and we discuss the extent to which nonperturbative physics can affect the NRQCD couplings. Finally, in Sec. VI, we summarize our results and discuss future prospects.

II. POWER-COUNTING RULES FOR NRQCD

NRQCD is an effective field theory which approximates ordinary relativistic QCD at low energies. In principle, the NRQCD action may be corrected to reproduce the exact results of QCD by including an infinite number of nonrenormalizable interactions. In practice, however, exact agreement is unnecessary: only a finite number of interactions are required to attain any desired accuracy. Some criterion is necessary to assess the importance of various interactions when designing the corrected action. In this section we categorize interactions by their effect on the energy spectrum of quarkonium states.

A. Building blocks for NRQCD

Correction terms $\delta\mathcal{L}(x)$ in the Lagrangian density of NRQCD contribute

$$\delta E = -\langle n| \int d^3x\, \delta\mathcal{L}(x) |n\rangle \tag{1}$$

to the energy of a quarkonium state $|n\rangle$. Since opera-

[2] A low-lying quarkonium state does decay, via the annihilation of the heavy quarks into gluons. The decay rate is relatively small and the decay mechanism has a negligible effect upon other properties of the hadron. Consequently, this decay mechanism is usually omitted in simulations.

tors are not normal-ordered in lattice simulations, there are cases where large contributions to δE involve contractions of two or more fields in a single term of $\delta\mathcal{L}(x)$. Such contributions have no bearing upon the relative importance of corrections since their effect is cancelled by shifts in the coupling constants of lower-dimension interactions. Thus we may ignore these contributions when estimating the importance of various terms. For the remaining contributions, each field and operator in $\delta\mathcal{L}(x)$ has a characteristic magnitude determined by the dynamics of the hadron.

The important dynamical scales for the nonrelativistic analysis of the ψ and Υ states are the typical momenta p and kinetic energies K of their quarks; these are of order 1–2 GeV and 500 MeV, respectively. If v is the quark velocity, the two scales are related to the quark mass M by

$$p \sim Mv, \quad K \sim Mv^2. \tag{2}$$

These determine the characteristic magnitudes of the fundamental fields and operators in NRQCD and allow us to estimate the (normal-ordered) contribution of any interaction to a quarkonium energy.

The continuum action for NRQCD is built from the fields and operators shown in Table I. We also list the estimated magnitude for each of these in terms of v and M. It is important to remember that it is the order in v rather than the dimension of an operator that determines its numerical importance. In this table, the quark field ψ and antiquark field χ have two spin components and three color components that transform in the fundamental representation. Combinations such as $\psi^\dagger\psi$ or $\chi^\dagger\psi$ are invariant under rotations and color transformations, while $\psi^\dagger\boldsymbol{\sigma}\psi$, for example, is a color singlet but rotates as a vector. The gauge fields have two color indices and transform in the adjoint representation. For example, the chromoelectric field is

$$\mathbf{E}(x) \equiv \mathbf{E}^a(x)\,T^a. \tag{3}$$

The generators T^a are normalized such that $\mathrm{Tr}(T^aT^b) = \delta^{ab}/2$. The combination $\psi^\dagger\mathbf{E}\psi$ is then a color-singlet vector field. Covariant derivatives act on the quark and gauge fields according to

$$\begin{aligned} D_t\psi(x) &\equiv [\partial_t + ig\phi(x)]\,\psi(x), \\ \mathbf{D}\psi(x) &\equiv [\boldsymbol{\nabla} - ig\mathbf{A}(x)]\,\psi(x), \\ D_tE_i(x) &\equiv \partial_tE_i(x) + i[g\phi(x), E_i(x)], \\ \mathbf{D}E_i(x) &\equiv \boldsymbol{\nabla}E_i(x) - i[g\mathbf{A}(x), E_i(x)]\,, \end{aligned} \tag{4}$$

where ϕ and $\mathbf{A}$ are the scalar and vector gauge potentials, and g is the coupling constant. The last definitions insure that the chain rule works properly for covariant derivatives. For example,

$$D(\mathbf{E}\psi) = (D\mathbf{E})\psi + \mathbf{E}(D\psi). \tag{5}$$

The non-Abelian electric and magnetic fields can be defined in terms of these covariant derivatives:

$$\begin{aligned} [D_t, \mathbf{D}]\,\psi &\equiv ig\mathbf{E}\psi, \\ [D_i, D_j]\,\psi &\equiv -ig\epsilon_{ijk}B^k\psi. \end{aligned} \tag{6}$$

The estimated sizes given in Table I follow from the properties of quarkonium states. For example, the number operator for (heavy) quarks,

$$\int d^3x\,\psi^\dagger(x)\,\psi(x), \tag{7}$$

has an expectation value very near 1 for a quarkonium meson. Since the quark in the meson is localized within a region $\Delta x \sim 1/p$, we estimate

$$\int d^3x \sim \frac{1}{p^3}\,, \tag{8}$$

and, therefore,

$$\psi^\dagger(x)\,\psi(x) \sim p^3\,, \tag{9}$$

that is, $\psi \sim p^{3/2}$. Similarly, the operator for kinetic energy,

$$\int d^3x\,\psi^\dagger(x)\,\frac{\mathbf{D}^2}{2M}\,\psi(x)\,, \tag{10}$$

has an expectation value of K by definition, and so the spatial covariant derivative acting on a quark field is of order

$$\mathbf{D} \sim (2\,M\,K)^{1/2} \sim p\,, \tag{11}$$

as expected.

Field equations can also be used to relate estimates for different operators. For example, the lowest-order field equation for the quark field,

$$\left(iD_t + \frac{\mathbf{D}^2}{2M}\right)\psi = 0\,, \tag{12}$$

implies that

$$D_t \sim \frac{\mathbf{D}^2}{2M} \sim K\,, \tag{13}$$

again as expected. If we specialize to Coulomb gauge, the gauge most natural for nonrelativistic systems, this equation becomes

TABLE I. The component fields and operators for the NRQCD action for heavy quarks. The estimated magnitude of each in a quarkonium state and in Coulomb gauge is given in terms of the quark mass M and typical velocity v.

Operator	Estimate	Description
ψ	$(Mv)^{3/2}$	Quark (annihilation) field
χ	$(Mv)^{3/2}$	Antiquark (creation) field
D_t	Mv^2	Gauge covariant time derivative
$\mathbf{D}$	Mv	Gauge covariant spatial derivative
$g\phi$	Mv^2	Scalar potential (Coulomb gauge)
$g\mathbf{A}$	Mv^3	Vector potential (Coulomb gauge)
$g\mathbf{E}$	M^2v^3	Chromoelectric field
$g\mathbf{B}$	M^2v^4	Chromomagnetic field

$$\left(i\partial_t - g\phi(x) + \frac{\nabla^2}{2M}\right)\psi \approx 0\,, \tag{14}$$

where we are neglecting the vector potential, which is small in this gauge, as discussed below. The potential energy that balances the kinetic energy and produces a bound system enters through the operator $g\phi$ and we expect that

$$g\phi(x) \sim K \tag{15}$$

in the Coulomb gauge.

This result can be checked against the field equation for ϕ (again neglecting the vector potential),

$$\nabla^2 g\phi(x) = -g^2\psi^\dagger(x)\psi(x)\,, \tag{16}$$

which implies that

$$g\phi(x) \sim \frac{1}{p^2}g^2p^3 \sim g^2p\,. \tag{17}$$

This is consistent with the previous estimate if the effective low-energy coupling strength is

$$\alpha_s \sim g^2 \sim v\,. \tag{18}$$

That the Coulomb-gauge vector potential in a quarkonium state is typically smaller than the scalar potential may be inferred from the field equation for the vector potential:

$$\left(\partial_t^2 - \nabla^2\right) g\mathbf{A} = \frac{g^2}{M}\psi^\dagger\nabla\psi + g\phi\nabla g\phi + \cdots\,. \tag{19}$$

Using the estimates given above, we see that

$$g\mathbf{A}(x) \sim \frac{1}{p^2}\left(\frac{g^2}{M}p^4 + pK^2\right) \sim vK, \tag{20}$$

which is smaller than the scalar potential by a factor of the quark velocity. Estimates for the non-Abelian electric and magnetic fields follow immediately from

$$\begin{aligned} g\mathbf{E} &= -\nabla g\phi + \cdots \sim pK, \\ g\mathbf{B} &= \nabla \times g\mathbf{A} + \cdots \sim K^2\,. \end{aligned} \tag{21}$$

In quarkonium, as expected for a nonrelativistic system, magnetic fields are smaller than electric fields by a factor of v.

These estimates are valid perturbatively, as in the analysis of positronium with NRQED, but are also consistent nonperturbatively. The essential ingredient in their derivations is the nonrelativistic nature of quark dynamics.

B. NRQCD interactions in the continuum

Equipped with the power-counting rules of the preceding section, we can enumerate terms for the quark action in NRQCD that are potentially important for quarkonium physics. The leading terms are those of the Schrödinger theory:

$$S_0 = \int d^4x\,\psi^\dagger(x)\left(iD_t + \frac{\mathbf{D}^2}{2M}\right)\psi(x). \tag{22}$$

Correction terms due to relativity and finite lattice spacing must respect the symmetries of the theory: gauge invariance, parity, rotational symmetry, unitarity, and so on. For example, the interaction $\psi^\dagger\mathbf{E}\cdot\boldsymbol{\sigma}\psi$, corresponding to an intrinsic electric dipole moment, is not allowed because it is odd under parity, while $\psi^\dagger\mathbf{B}\cdot\boldsymbol{\sigma}\psi$ is even under parity and so is allowed. Charge-conjugation invariance requires that the total action be invariant under the interchange $\psi \leftrightarrow \chi$. Thus the antiquark action can be obtained directly from the quark action.

Correction terms must also be local. This, combined with the fact that our theory needs only to be accurate to 10%, severely restricts the number of interactions. For example, the interaction $\psi^\dagger\mathbf{B}^2\psi/M^3$ is consistent with required symmetries and so must appear in the NRQCD action. But it is unnecessary for our calculations because it is suppressed by v^6 ($\approx 10^{-3}$ for Υ's) relative to the leading terms in the action.

Ignoring spin splittings for the moment, only corrections that are suppressed by v^2 relative to the leading terms are needed to achieve accuracy to 10%, at least for Υ's. The only such terms bilinear in the quark field are the order-v^2 corrections

$$\begin{aligned} \delta\mathcal{L}_{\text{bilinear}} \equiv\ & c_1\frac{1}{M^3}\psi^\dagger\mathbf{D}^4\psi \\ & + c_2\frac{g}{M^2}\psi^\dagger(\mathbf{D}\cdot\mathbf{E} - \mathbf{E}\cdot\mathbf{D})\psi \\ & + c_3\frac{ig}{M^2}\psi^\dagger\boldsymbol{\sigma}\cdot(\mathbf{D}\times\mathbf{E} - \mathbf{E}\times\mathbf{D})\psi \\ & + c_4\frac{g}{M}\psi^\dagger\boldsymbol{\sigma}\cdot\mathbf{B}\psi\,. \end{aligned} \tag{23}$$

In this and subsequent equations, $\mathbf{D}$ acts on all fields to its right. The dimensionless coefficients $c_1, \ldots, c_4$ are functions of the running coupling constant $\alpha_s(\pi/a)$ and aM.

Note that terms involving time derivatives of the quark field, such as $\psi^\dagger D_t^2\psi$, are not included. Such terms greatly complicate the numerical evaluation of quark propagators. We may avoid them here by suitably redefining the quark field so that factors of iD_t are in effect replaced by factors of $-\mathbf{D}^2/2M$, in accordance with the field equation for ψ,

$$iD_t\psi(x) \approx \frac{-\mathbf{D}^2}{2M}\psi(x)\,. \tag{24}$$

These transformations do not affect masses, on-shell scattering amplitudes, or other physical quantities.

In addition to the bilinear terms, there are four-fermion contact interactions involving a quark and antiquark:

$$\begin{aligned} \delta\mathcal{L}_{\text{contact}} \equiv\ & d_1\frac{1}{M^2}\psi^\dagger\chi\chi^\dagger\psi \\ & + d_2\frac{1}{M^2}\psi^\dagger\boldsymbol{\sigma}\chi\cdot\chi^\dagger\boldsymbol{\sigma}\psi\,. \end{aligned} \tag{25}$$

These appear to be down by only a single power of v. However, similar interactions do not occur in relativistic continuum QCD, and therefore such terms can occur

here only to one-loop order and beyond. Thus the coefficients d_1 and d_2 are both of order $\alpha_s^2(\pi/a)$, making these contact interactions significantly less important than the bilinear interactions considered above. Contact interactions also occur between pairs of quarks, but these can only affect heavy-quark baryons. Four-fermion operators can also couple to colored states:

$$\delta\mathcal{L}_{\rm color} \equiv d_3 \frac{1}{M^2} \sum_a \psi^\dagger T^a \chi \chi^\dagger T^a \psi + d_4 \frac{1}{M^2} \sum_a \psi^\dagger T^a \boldsymbol{\sigma} \chi \cdot \chi^\dagger T^a \boldsymbol{\sigma} \psi \,, \tag{26}$$

where d_3 and d_4 are of order $\alpha_s^2(\pi/a)$. Color-singlet mesons are affected by these interactions, since the meson can become colored by emitting a virtual gluon. Gluon emission, however, is suppressed by v^2, so these interactions are again not as important as the bilinear terms in Eq. (23).

Nontrivial spin dependence first appears in the bilinear correction terms of Eq. (23), so that spin splittings in quarkonium meson families are suppressed by v^2. A 10% determination of these splittings therefore requires the retention of spin-dependent interactions suppressed by v^4. The additional quark-bilinear terms required to this order are of three sorts: permutations of the operators $\psi^\dagger\boldsymbol{\sigma}\psi$, $\mathbf{B}$, and two $\mathbf{D}$'s; permutations of the operators $\psi^\dagger\boldsymbol{\sigma}\psi$, $\mathbf{D}\times\mathbf{E}$, and two $\mathbf{D}$'s; and the operator $\psi^\dagger\boldsymbol{\sigma}\cdot\mathbf{E}\times\mathbf{E}\psi$, which is nonzero in non-Abelian theories. Of these, only three interactions occur in our treatment:

$$\delta\mathcal{L}_{\rm spin} \equiv f_1 \frac{g}{M^3} \psi^\dagger \{\mathbf{D}^2, \boldsymbol{\sigma}\cdot\mathbf{B}\}\psi + f_2 \frac{ig}{M^4} \psi^\dagger \{\mathbf{D}^2, \boldsymbol{\sigma}\cdot(\mathbf{D}\times\mathbf{E} - \mathbf{E}\times\mathbf{D})\}\psi + f_3 \frac{ig^2}{M^3} \psi^\dagger \boldsymbol{\sigma}\cdot\mathbf{E}\times\mathbf{E}\psi \,. \tag{27}$$

The power-counting rules indicate that spin splittings in quarkonium systems should be smaller than splittings between radial and orbital excitations. This is a familiar feature of the experimental data. The ψ'–ψ and Υ'–Υ mass splittings are both around 600 MeV. Our analysis indicates that spin splittings should be smaller than this by a factor of v^2; that is, approximately 180 MeV for ψ's and 60 MeV for Υ's. In fact experiments show that the p-state hyperfine splitting, $\chi(2^{++})$–$\chi(0^{++})$, is 141 MeV for the ψ family, and 34 MeV for Υ's. The sizes of these splittings are consistent with our expectations, and show clear evidence of appropriate scaling with v^2. The s-state hyperfine splitting between the ψ and η_c of about 117 MeV is also consistent. These data reinforce our confidence in the power-counting rules, and in the utility of a nonrelativistic framework for studying these mesons.

One final source of corrections comes from vacuum polarization of heavy quarks. These modify the gluon action at order $\alpha_s(M)\,v^2$ and so can probably be ignored at the 10% level. Such corrections are essentially relativistic in character and should not be analyzed using NRQCD. They are easily computed using continuum perturbation theory.

III. RELATIVISTIC CORRECTIONS

The corrections to the continuum NRQCD action required by relativity were enumerated in Sec. II. Our task now is to find values for the coupling constants multiplying these operators such that the predictions of NRQCD agree with those of ordinary QCD through order v^2. Since the coupling constants have perturbative expansions, we will determine them by matching perturbative results in the two theories. Here we work only to lowest order, or tree level, in perturbation theory. Higher-order corrections will be discussed in Sec. V.

A. Kinetic terms

The simplest correction follows immediately from the formula for the relativistic energy of a noninteracting quark:

$$\sqrt{\mathbf{p}^2 + M^2} \approx M + \frac{\mathbf{p}^2}{2M} - \frac{\mathbf{p}^4}{8M^3} \,. \tag{28}$$

This implies a correction term, appropriately gauged, of the form

$$\delta\mathcal{L}_K = \frac{1}{8M^3}\psi^\dagger \mathbf{D}^4 \psi \,, \tag{29}$$

which fixes $c_1 = \frac{1}{8}$ in Eq. (23).

B. Electric couplings

Most of the corrections from Sec. II involving the chromoelectric field are linear in $g\mathbf{E}$. We compute these terms by examining the order-g amplitude T_E for scattering a quark off a static electric field in QCD:

$$T_E(\mathbf{p},\mathbf{q}) = \overline{u}(\mathbf{q})\gamma^0\, g\phi(\mathbf{q}-\mathbf{p})\, u(\mathbf{p}) \,, \tag{30}$$

with ϕ the scalar potential. We are interested in matching this result at small v to that obtained in NRQCD, and so must expand it in powers of $\mathbf{q}/M$ and $\mathbf{p}/M$. The Dirac spinor, normalized nonrelativistically with $u^\dagger u = 1$, is

$$u(\mathbf{p}) = \left(\frac{E_p + M}{2E_p}\right)^{\frac{1}{2}} \begin{bmatrix} \psi \\ \dfrac{\boldsymbol{\sigma}\cdot\mathbf{p}}{E_p + M}\psi \end{bmatrix} \,, \tag{31}$$

with $E_p \equiv \sqrt{\mathbf{p}^2 + M^2}$ and ψ a two-component spinor. Substituting this expression in Eq. (30) we obtain

$$T_E(\mathbf{p},\mathbf{q}) = \sqrt{\frac{(E_p+M)(E_q+M)}{4E_pE_q}} \times \psi^\dagger \left[1 + \frac{\mathbf{p}\cdot\mathbf{q} + i\boldsymbol{\sigma}\cdot\mathbf{q}\times\mathbf{p}}{(E_q+M)(E_p+M)}\right] g\phi(\mathbf{q}-\mathbf{p})\,\psi \equiv S_E(\mathbf{p},\mathbf{q}) + V_E(\mathbf{p},\mathbf{q}) \,, \tag{32}$$

where S_E denotes the scalar part of the amplitude, independent of $\boldsymbol{\sigma}$, and V_E is the spin-dependent term. Expanding both S_E and V_E to second order in $\mathbf{p}/M$ and $\mathbf{q}/M$,

$$S_E(\mathbf{p},\mathbf{q}) = \left(1 - \frac{(\mathbf{p}-\mathbf{q})^2}{8M^2}\right) \psi^\dagger\, g\phi(\mathbf{q}-\mathbf{p})\, \psi,$$

$$V_E(\mathbf{p},\mathbf{q}) = \left(\frac{i}{4M^2} - \frac{3i}{32M^4}(\mathbf{p}^2+\mathbf{q}^2)\right) \times \psi^\dagger\, \boldsymbol{\sigma}\cdot\mathbf{q}\times\mathbf{p}\, g\phi(\mathbf{q}-\mathbf{p})\, \psi. \tag{33}$$

By computing the same process in NRQCD and comparing with the QCD result at low momentum, it is possible to determine which operators must appear in the NRQCD Lagrangian and to fix their coefficients. The first term in the lowest-order NRQCD action, Eq. (22), predicts a scattering amplitude $\psi^\dagger\, g\phi(\mathbf{q}-\mathbf{p})\,\psi$. This corresponds to the first term in S_E. The remaining terms in S_E and V_E can only be included by adding the new interactions

$$\begin{aligned}\delta\mathcal{L}_E = {} & \frac{g}{8M^2}\psi^\dagger(\mathbf{D}\cdot\mathbf{E} - \mathbf{E}\cdot\mathbf{D})\psi \\ & + \frac{ig}{8M^2}\psi^\dagger\,(\boldsymbol{\sigma}\cdot\mathbf{D}\times\mathbf{E} - \boldsymbol{\sigma}\cdot\mathbf{E}\times\mathbf{D})\,\psi \\ & + \frac{3ig}{64M^4}\psi^\dagger\{\mathbf{D}^2,\, \boldsymbol{\sigma}\cdot\mathbf{D}\times\mathbf{E} - \boldsymbol{\sigma}\cdot\mathbf{E}\times\mathbf{D}\}\psi \end{aligned} \tag{34}$$

to the NRQCD action. The coefficients c_2 and c_3 in Eq. (23) are therefore $\frac{1}{8}$, while f_2 in Eq. (27) is $\frac{3}{64}$.

C. Magnetic couplings

Similarly, we determine the operators linear in $\mathbf{B}$ by calculating the amplitude for the scattering of a quark off a static vector potential $\mathbf{A}(\mathbf{x})$. The time independence of $\mathbf{A}(\mathbf{x})$ guarantees that there is no electric component. It also enforces the conservation of the quark energy.

The amplitude is

$$T_B(\mathbf{p},\mathbf{q}) = -\overline{u}(\mathbf{q})\boldsymbol{\gamma}\cdot g\mathbf{A}(\mathbf{q}-\mathbf{p})u(\mathbf{p}), \tag{35}$$

where $\mathbf{p}^2 = \mathbf{q}^2$. Expanding in $\mathbf{p}/M$ and employing energy conservation,

$$\begin{aligned} T_B(\mathbf{p},\mathbf{q}) &= -\frac{g}{2M}\left(1 - \frac{\mathbf{p}^2}{2M^2}\right) \times \psi^\dagger\,[(\mathbf{p}+\mathbf{q})\cdot\mathbf{A} + i\boldsymbol{\sigma}\cdot\mathbf{A}\times(\mathbf{p}-\mathbf{q})]\,\psi \\ &\equiv S_B(\mathbf{p},\mathbf{q}) + V_B(\mathbf{p},\mathbf{q}). \end{aligned} \tag{36}$$

The spin-independent term $S_B(\mathbf{p},\mathbf{q})$ arises in NRQCD from the terms linear in $g\mathbf{A}$ which appear in the kinetic energy part of the action, Eqs. (22) and (29). The spin-dependent term V_B must be generated by the new interactions

$$\begin{aligned}\delta\mathcal{L}_B = {} & \frac{g}{2M}\psi^\dagger\boldsymbol{\sigma}\cdot\mathbf{B}\psi \\ & + \frac{g}{8M^3}\psi^\dagger\{\mathbf{D}^2,\, \boldsymbol{\sigma}\cdot\mathbf{B}\}\psi, \end{aligned} \tag{37}$$

so that $c_4 = \frac{1}{2}$ and $f_1 = \frac{1}{8}$ in Eq. (23) and Eq. (27).

D. Bilinears in $F_{\mu\nu}$

The interaction $\psi^\dagger\,\boldsymbol{\sigma}\cdot\mathbf{E}\times\mathbf{E}\,\psi$, which contributes to spin splittings, is the only bilinear in $F_{\mu\nu}$ that contributes to the accuracy desired. To fix the coefficient of this operator [f_3 in Eq. (27)], we calculate the amplitude for double scattering of a quark off an external static electric field. In QCD, it is

$$\begin{aligned} T_{EE}(\mathbf{p}_1,\mathbf{p}_2) = -i\int & \frac{d^3q_1}{(2\pi)^3}\frac{d^3q_2}{(2\pi)^3}(2\pi)^3\delta^3(\mathbf{q}_1+\mathbf{q}_2+\mathbf{p}_1-\mathbf{p}_2) \\ & \times\overline{u}(\mathbf{p}_2)\gamma^0\, g\phi(\mathbf{q}_2)\,\frac{i}{(\not{p}_1+\not{q}_1) - M + i\epsilon}\, g\phi(\mathbf{q}_1)\,\gamma^0 u(\mathbf{p}_1). \end{aligned} \tag{38}$$

This same process must be computed in NRQCD, and compared to an expansion of Eq. (38) at small $\mathbf{p}/M$. This comparison is simplified by using the identity

$$\frac{1}{\not{k} - M} = \sum_s \left[\frac{u_s(\mathbf{k})\,\overline{u}_s(\mathbf{k})}{k^0 - E} + \frac{v_s(-\mathbf{k})\,\overline{v}_s(-\mathbf{k})}{k^0 + E}\right] \tag{39}$$

for the fermion propagator, to break T_{EE} into two terms before expanding. NRQCD, with the terms computed thus far, reproduces the first term containing $u\,\overline{u}/(k^0-E)$ to the required order in v, using vertices derived from the interactions of Eq. (34). These were designed to match the matrix element of Eq. (30), $\overline{u}\gamma^0\, g\phi\, u$, and the first term of Eq. (39) contributes the same matrix elements to each of the vertices of the QCD diagram. The energy denominator

$$\begin{aligned}\frac{1}{k^0 - E} \sim {} & \frac{1}{\tilde{k}^0 - \mathbf{k}^2/2M} \\ & - \frac{1}{\tilde{k}^0 - \mathbf{k}^2/2M}\left(\frac{\mathbf{k}^4}{8M^3}\right)\frac{1}{\tilde{k}^0 - \mathbf{k}^2/2M}, \end{aligned} \tag{40}$$

with the kinetic energy $\tilde{k}^0 \equiv k^0 - M$, is reproduced in NRQCD by its nonrelativistic propagator and the kinetic term correction of Sec. III A.

The second part of T_{EE}, when expanded, introduces a term of an entirely different character. To lowest order in v, for low-momentum external gluons, the antiquark propagator is just $(2M)^{-1}$, so this part behaves as a local seagull interaction. This contributes to Eq. (38)

$$\begin{aligned} -\int & \frac{d^3q_1}{(2\pi)^3}\frac{d^3q_2}{(2\pi)^3}(2\pi)^3\delta^3(\mathbf{q}_1+\mathbf{q}_2+\mathbf{p}_1-\mathbf{p}_2) \\ & \times\frac{1}{8M^3}\psi^\dagger\, g\phi(\mathbf{q}_2)\,[\mathbf{q}_1\cdot\mathbf{q}_2 - i\boldsymbol{\sigma}\cdot\mathbf{q}_1\times\mathbf{q}_2]g\phi(\mathbf{q}_1)\,\psi. \end{aligned} \tag{41}$$

In order to obtain the same result with NRQCD, we must include the new interaction

$$\delta\mathcal{L}_{EE} = -\frac{g^2}{8M^3}\psi^\dagger\,[\mathbf{E}\cdot\mathbf{E} + i\boldsymbol{\sigma}\cdot\mathbf{E}\times\mathbf{E}]\psi\,. \tag{42}$$

To the order to which we are working only the second term, which contributes to spin splittings at order v^4, must be retained. So $f_3 = -\frac{1}{8}$ in Eq. (27), and we have determined all relevant tree-level coefficients of the NRQCD Lagrangian.

E. The NRQCD continuum Lagrangian

The Lagrangian for continuum NRQCD in Minkowski space is

$$\mathcal{L}_{\rm NRQCD} \equiv i\psi^\dagger D_t\psi + \psi^\dagger\frac{\mathbf{D}^2}{2M}\psi + \delta\mathcal{L}_K + \delta\mathcal{L}_E + \delta\mathcal{L}_B + \delta\mathcal{L}_{EE}\,, \tag{43}$$

where the relativistic corrections are defined in Eqs. (29), (34), (37), and (42), respectively. We have not included in the Lagrangian a mass term $M\psi^\dagger\psi$ because in a nonrelativistic framework it only fixes the zero-point energy and has no effect on mass splittings, wave functions, and so on. As an independent check, we performed the systematic but lengthy calculation of the Lagrangian in Eq. (43) using the Foldy-Wouthuysen-Tani transformation [5]. This transformation is not directly applicable beyond the tree level. However, perturbative corrections to the various coefficients may be computed by comparing amplitudes, as in Secs. III B–III D, but including loop corrections.

Finally, we note that for lattice simulations we will need the Euclidean action. This is obtained from the Minkowski theory defined by Eq. (43) by keeping track of how the three-dimensional vectors and scalars are defined in terms of Lorentz-covariant quantities. Under Wick rotation the zero component of contravariant vectors rotates as the time coordinate,

$$x^0_{(M)} = -ix^0_{(E)}\,, \tag{44}$$

while the zero component of covariant vectors rotates as the time derivative:

$$\partial_0^{(M)} = +i\partial_0^{(E)}\,. \tag{45}$$

Spatial components of all four-vectors are unchanged. Wick rotation changes the sign of the $(0,0)$ component of the metric tensor, so that the usual Minkowski metric $\eta_{\mu\nu} \equiv \mathrm{diag}(1,-1,-1,-1)$ rotates to the negative of the identity matrix. One then has to extract this minus sign from scalar products in order to work with the usual positive-definite Euclidean metric. Our definitions for the basic operators appearing in Eq. (43) are

$$\begin{aligned} D_0^{(M)} &= +iD_0^{(E)}, \\ \phi_{(M)} &= -i\phi_{(E)}, \\ E^i_{(M)} &= -iE^i_{(E)}\,, \end{aligned} \tag{46}$$

while other fields are unaffected.

IV. LATTICE NRQCD

A. Leading order

NRQCD is readily reformulated on a discrete spacetime lattice. As usual, quark fields $\psi(x)$ are defined at the nodes of the lattice, while gauge fields are represented by unitary matrices $U_{x,\mu}$ defined on the links joining neighboring nodes. Covariant derivatives are replaced by forward, backward, or centered differences,

$$\begin{aligned} a\Delta^{(+)}_\mu\psi(x) &\equiv U_{x,\mu}\,\psi(x+a\hat{\mu}) - \psi(x), \\ a\Delta^{(-)}_\mu\psi(x) &\equiv \psi(x) - U^\dagger_{x-a\hat{\mu},\mu}\,\psi(x-a\hat{\mu}), \\ \Delta^{(\pm)} &\equiv \tfrac{1}{2}(\Delta^{(+)} + \Delta^{(-)})\,, \end{aligned} \tag{47}$$

depending upon the details of the interaction, while the Laplacian becomes

$$\boldsymbol{\Delta}^{(2)} \equiv \sum_i \Delta^{(+)}_i\Delta^{(-)}_i = \sum_i \Delta^{(-)}_i\Delta^{(+)}_i. \tag{48}$$

The field $F_{\mu\nu}(x)$ is efficiently represented by cloverleaf operators defined at the nodes of the lattice [6]:

$$gF^{(c)}_{\mu\nu}(x) = -\frac{1}{4a^2}\sum_{P(x,\mu\nu)}\mathcal{I}[U_{P(x,\mu\nu)}]\,, \tag{49}$$

where the sum is over all plaquettes P in the (μ,ν) plane containing the site x. U_P is the product of link matrices on P, counterclockwise about $\hat{\mu}\times\hat{\nu}$, as depicted in Fig. 1. The operator $\mathcal{I}$ is defined as

$$\mathcal{I}[M] \equiv \frac{M - M^\dagger}{2i} - \frac{1}{3}\,\mathrm{Im}(\mathrm{Tr}\,M)\,. \tag{50}$$

Covariant derivatives of $F_{\mu\nu}$ are represented by the differences

$$\begin{aligned} a\Delta^{(+)}_\rho F^{(c)}_{\mu\nu}(x) &\equiv U_{x,\rho}\,F^{(c)}_{\mu\nu}(x+a\hat{\rho})U^\dagger_{x,\rho} - F^{(c)}_{\mu\nu}(x), \\ a\Delta^{(-)}_\rho F^{(c)}_{\mu\nu}(x) &\equiv F^{(c)}_{\mu\nu}(x) \\ &\quad - U^\dagger_{x-a\hat{\rho},\rho}F^{(c)}_{\mu\nu}(x-a\hat{\rho})U_{x-a\hat{\rho},\rho}\,. \end{aligned} \tag{51}$$

All terms in the NRQCD action are built with these elements.

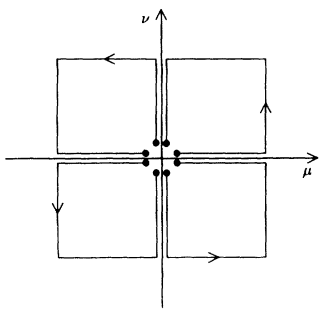

FIG. 1. Wilson lines appearing in the cloverleaf definition of the field $F_{\mu\nu}$.

Focusing on the leading-order terms, we may define a series of lattice actions for NRQCD,

$$S_0^{(n)} = a^3 \sum_x \psi^\dagger(x)\psi(x) - a^3 \sum_x \psi^\dagger(x+a\hat{t}) \left(1 - \frac{aH_0}{2n}\right)^n \times U_{x,t}^\dagger \left(1 - \frac{aH_0}{2n}\right)^n \psi(x), \quad (52)$$

where n is a positive integer and H_0 is the kinetic energy operator

$$H_0 \equiv -\frac{\Delta^{(2)}}{2M}. \quad (53)$$

The quark Green's function for such a theory satisfies a simple evolution equation

$$G(\mathbf{x}, t+a) = \left(1 - \frac{aH_0}{2n}\right)^n U_{x,t}^\dagger \left(1 - \frac{aH_0}{2n}\right)^n \times G(\mathbf{x}, t) + \delta_{\mathbf{x},0}\delta_{t+a,0}, \quad (54)$$

where $G(\mathbf{x}, t)$ vanishes for $t < 0$. This evolution equation differs from others that have been suggested. It is symmetric with respect to time reversal, unlike that of [2]. Also, as we will see, it leads to a wave-function renormalization much smaller than that of [3].

The parameter n was introduced to prevent instabilities at large momenta due to the kinetic energy operator [2]. The Green's function defined by Eq. (54) blows up if $\max(aH_0/2n) \geq 2$, and so n must be large enough to avoid this. Neglecting gluons, this implies that $n > 3/(2Ma)$ is required for stability; gluonic effects reduce the $\frac{3}{2}$ to something closer to 1.15 for $\beta \approx 6$ [3]. Thus, at $\beta = 6$, $n = 1$ suffices for b quarks, while $n = 2$ is needed for c quarks. Larger n's may be required as β is increased and a decreases.

B. Lattice spacing errors

The finite spacing of the lattice introduces new systematic errors into NRQCD. Errors associated with the temporal spacing a_t are typically of order $a_t\langle K\rangle$, while those due to the spatial lattice are of order $a_x^2\langle \mathbf{p}^2\rangle$. The two tend to be roughly comparable since usually $a_x = a_t \approx 1/M$. Both must be removed if we are to achieve high precision.

Errors due to the finite lattice spacing are removed by adding new interactions to the Lagrangian, just as $O(v^2)$ errors were removed. As in that case, we could compute the necessary corrections by matching perturbative scattering amplitudes in lattice NRQCD with those in continuum QCD. However, at tree level, it is simpler to correct the individual components from which the lattice action is built ($\Delta^{(2)}$, $\mathbf{E}$, $\mathbf{B}$,...) so that they more accurately reproduce the effects of their continuum analogues. This is the approach we will follow here.

To compare the effects of lattice operators with those of continuum operators we need some way to relate fields on the lattice to those in the continuum. For the quarks, we simply identify the lattice field at a site with the continuum field at the same space-time point. For the gluons, gauge invariance requires that the link operator be related to the continuum gauge field through the path-ordered exponential of a line integral,

$$U_{x,\mu} \equiv P \exp\left[-ig \int_x^{x+a\hat{\mu}} A \cdot dy\right], \quad (55)$$

where the scalar product is taken with the positive Euclidean metric. The simplest choice of path for the integral is a straight line joining x to $x + a\hat{\mu}$; other choices lead to the same final results but give more complicated $O(a)$ corrections. With this mapping from lattice variables to continuum variables, we can now correct each of the lattice operators.

1. Spatial derivatives

Given relation (55), the action of the lattice difference operators on continuum fields is specified by

$$a\Delta_i^{(+)} \equiv \exp(aD_i) - 1 = aD_i + \frac{a^2}{2}D_i^2 + \cdots, \quad a\Delta_i^{(-)} \equiv 1 - \exp(-aD_i) = aD_i - \frac{a^2}{2}D_i^2 + \cdots. \quad (56)$$

These are just gauge-covariant extensions of the obvious $g = 0$ relations. By combining these expansions we obtain an improved difference operator that reproduces the effects of D_i through order a^4:

$$\tilde{\Delta}_i^{(\pm)} \equiv \Delta_i^{(\pm)} - \frac{a^2}{6}\Delta_i^{(+)}\Delta_i^{(\pm)}\Delta_i^{(-)}. \quad (57)$$

Similarly we may define an improved lattice Laplacian that is also accurate to order a^4:

$$\tilde{\Delta}^{(2)} = \Delta^{(2)} - \frac{a^2}{12}\sum_i \left[\Delta_i^{(+)}\Delta_i^{(-)}\right]^2. \quad (58)$$

2. Temporal derivative

Temporal and spatial derivatives enter NRQCD differently because the theory is nonrelativistic. One consequence is that quark propagation is governed by a Schrödinger equation with a single time derivative. The calculation of quark Green's functions is therefore an initial value problem, which is much less costly to solve numerically than the boundary value problem dictated by the Dirac equation. If we improve the time derivative operator as we did for spatial derivatives, this simplification is lost, as we would need to introduce higher-order time derivatives.

To find an alternative, we examine the evolution equation for the quark Green's function, Eq. (54). Neglecting the gauge field for the moment, this equation may be written (for $t > 0$)

$$G(\mathbf{x}, t+a) = \left(1 - \frac{aH_0}{2n}\right)^{2n} G(\mathbf{x}, t)$$
$$= e^{-aH_{\rm eff}} G(\mathbf{x}, t)\,, \tag{59}$$

where the effective Hamiltonian

$$H_{\rm eff} \equiv -\frac{2n}{a} \ln\left(1 - \frac{aH_0}{2n}\right)$$
$$= H_0 + \frac{a}{4n} H_0^2 + \cdots\,. \tag{60}$$

The order-a term in the effective Hamiltonian cancels if we replace H_0 by

$$\tilde{H}_0 \equiv H_0 - \frac{a}{4n} H_0^2\,. \tag{61}$$

Making this replacement in the full evolution equation [Eq. (54)] removes the leading error due to our lattice approximation of the temporal derivative.[3] The resulting theory is equivalent to what would have been obtained by improving the temporal derivative along the lines presented in the previous section; the two theories are related by a redefinition of the quark field, and so give the same results for energy levels, on-shell scattering amplitudes, and other physical quantities.

3. Electric and magnetic fields

The lattice cloverleaf field $F_{\mu\nu}^{(c)}(x)$ [Eq. (49)] is equal to the continuum field $F_{\mu\nu}(x)$ up to corrections of order a^2. Our power-counting analysis (Sec. II) implies that only corrections linear in $F_{\mu\nu}$ are important. Such corrections are the same in an Abelian theory as they are in QCD, so we simplify the analysis by focusing on the Abelian case.

In the Abelian theory, where the operator $\mathcal{I}$ just takes the imaginary part, the cloverleaf field is

$$a^2 g F_{\mu\nu}^{(c)}(x) = -\,\mathrm{Im}\left(1 - \frac{ig}{4}\oint_{(2\times 2)} A\cdot dy + \cdots\right)$$
$$= \frac{g}{4}\int_{(2\times 2)} (\partial_\mu A_\nu - \partial_\nu A_\mu)\, dy^\mu \wedge dy^\nu + O(a^6)$$
$$= a^2 g F_{\mu\nu}(x) + \frac{a^4}{6}(\partial_\mu^2 + \partial_\nu^2) g F_{\mu\nu}(x) + O(a^6)\,, \tag{62}$$

where the surface integral is over the (2×2) plaquette in the (μ, ν) plane centered at x. The a^4 term comes from the second-order term in the Taylor expansion of $F_{\mu\nu}$ around point x. The non-Abelian generalization of this result is obtained by replacing derivatives with covariant derivatives.

By subtracting the lattice version of the $O(a^2)$ error,

$$g\tilde{F}_{\mu\nu}^{(c)}(x) = g F_{\mu\nu}^{(c)}(x) - \frac{a^2}{6}\left[\Delta_\mu^{(+)}\Delta_\mu^{(-)} + \Delta_\nu^{(+)}\Delta_\nu^{(-)}\right] g F_{\mu\nu}^{(c)}(x)\,, \tag{63}$$

we have a definition accurate to $O(a^4)$. Expanding the lattice derivatives as in Eq. (51), we obtain finally

$$g\tilde{F}_{\mu\nu}^{(c)}(x) = \tfrac{5}{3} g F_{\mu\nu}^{(c)}(x) - \tfrac{1}{6}\left[U_{x,\mu} g F_{\mu\nu}^{(c)}(x + a\hat{\mu}) U_{x,\mu}^\dagger + U_{x-a\hat{\mu},\mu}^\dagger g F_{\mu\nu}^{(c)}(x - a\hat{\mu}) U_{x-a\hat{\mu},\mu} - (\mu \Leftrightarrow \nu)\right]. \tag{64}$$

We have verified that $\tilde{F}_{\mu\nu}^{(c)}$ reproduces the continuum $F_{\mu\nu}$ to $O(a^4)$ directly in the non-Abelian theory using techniques described in the Appendix.

4. The gauge field action

The gluon action has lattice spacing errors as large as those of the nonrelativistic quark action. A great deal of sophisticated work has been done on improving the gauge field action, dealing mainly with one-loop contributions [7]. For us, however, a straightforward improvement of the classical action is all that is required. In particular, corrections involving nonplanar loops are not needed. This greatly simplifies our analysis.

Power counting indicates that the non-Abelian and Abelian corrections have the same form. By Stokes' theorem, a single Abelian plaquette centered at point x is related to the continuum field tensor by

$$U_P(x) = \exp\Big[-iga^2 F_{\mu\nu}(x)$$
$$-ig\frac{a^4}{24}(\partial_\mu^2 + \partial_\nu^2) F_{\mu\nu}(x) + O(a^6)\Big]\,, \tag{65}$$

and the usual lattice Lagrangian is

[3] Only the kinetic part of the Hamiltonian needs fixing here. The gauge-potential part is automatically exponentiated since the gauge fields enter through the link variables $U_{x,\mu}$.

$$\frac{1}{2g^2a^4}\mathrm{Re}\,[U_P(x)-1] = -\frac{1}{4}F_{\mu\nu}^2(x) - \frac{a^2}{48}F_{\mu\nu}(x)(\partial_\mu^2+\partial_\nu^2)F_{\mu\nu}(x) + O(a^4)\,. \tag{66}$$

The non-Abelian generalization is straightforward; the key result is that the corrections are of order a^2.

A simple scaling argument allows us to correct the non-Abelian action. The usual Lagrangian involves a sum over all four (1×1) plaquettes at a site x,

$$\mathcal{L}_G(x) = \frac{1}{4g^2a^4}\sum_{P(1\times1)}\mathrm{Tr}\left[\mathcal{R}\left(U_{P(1\times1)}\right)\right], \tag{67}$$

where

$$\mathcal{R}(M) \equiv \frac{M+M^\dagger}{2} - 1\,. \tag{68}$$

From the discussion above,

$$\mathcal{L}_G = \mathcal{L}_G^{\mathrm{cont}} + a^2\,\delta\mathcal{L}_G + O(a^4)\,, \tag{69}$$

where $\mathcal{L}_G^{\mathrm{cont}}$ is the continuum Lagrangian. An acceptable Lagrangian may also be constructed from (2×2) plaquettes, and its a dependence follows from Eqs. (67) and (69), with the replacement $a\to 2a$:

$$\mathcal{L}_G^{(2\times2)}(x) = \frac{1}{64g^2a^4}\sum_{P(2\times2)}\mathrm{Tr}\left[\mathcal{R}\left(U_{P(2\times2)}\right)\right] = \mathcal{L}_G^{\mathrm{cont}} + 4a^2\,\delta\mathcal{L}_G + O(a^4)\,. \tag{70}$$

By combining these two Lagrangians, we obtain a gluon Lagrangian that is accurate to order a^4:

$$\tilde{\mathcal{L}}_G = \tfrac{1}{3}\left(4\mathcal{L}_G - \mathcal{L}_G^{(2\times2)}\right) = -\tfrac{1}{2}\mathrm{Tr}\left[F_{\mu\nu}^2\right] + O(a^4)\,. \tag{71}$$

Again, this result may be confirmed directly in the non-Abelian theory by means of the techniques described in the Appendix.

C. A corrected evolution equation

The leading-order evolution equation, Eq. (54), for the quark Green's function is readily generalized to include relativistic and finite a corrections. We choose the full evolution equation to be

$$G(\mathbf{x},t+a) = \left(1-\frac{a\tilde{H}_0}{2n}\right)^n\left(1-\frac{a\,\delta H}{2}\right)U_{x,t}^\dagger\left(1-\frac{a\,\delta H}{2}\right)\left(1-\frac{a\tilde{H}_0}{2n}\right)^n G(\mathbf{x},t) \tag{72}$$

for $t>0$. Here we have corrected the leading kinetic energy operator for finite lattice spacing errors as in Eqs. (58) and (61) so that

$$\tilde{H}_0 \equiv -\frac{\tilde{\mathbf{\Delta}}^{(2)}}{2M} - \frac{a}{4n}\frac{(\mathbf{\Delta}^{(2)})^2}{4M^2}\,. \tag{73}$$

Further, a straightforward transcription of the relativistic corrections into lattice variables gives, for the spin-independent corrections,

$$\delta H_{K,v^2} \equiv -\frac{(\mathbf{\Delta}^{(2)})^2}{8M^3}, \tag{74}$$

$$\delta H_{v^2} \equiv \frac{ig}{8M^2}\left(\mathbf{\Delta}^{(\pm)}\cdot\mathbf{E} - \mathbf{E}\cdot\mathbf{\Delta}^{(\pm)}\right), \tag{75}$$

and, for the spin-dependent terms,

$$\delta H_{\mathrm{spin}} \equiv -\frac{g}{8M^2}\boldsymbol{\sigma}\cdot\left(\tilde{\mathbf{\Delta}}^{(\pm)}\times\tilde{\mathbf{E}} - \tilde{\mathbf{E}}\times\tilde{\mathbf{\Delta}}^{(\pm)}\right) - \frac{g}{2M}\boldsymbol{\sigma}\cdot\tilde{\mathbf{B}}, \tag{76}$$

$$\delta H_{\mathrm{spin},v^2} \equiv -\frac{g}{8M^3}\{\mathbf{\Delta}^{(2)},\boldsymbol{\sigma}\cdot\mathbf{B}\} - \frac{3g}{64M^4}\{\mathbf{\Delta}^{(2)},\boldsymbol{\sigma}\cdot(\mathbf{\Delta}^{(\pm)}\times\mathbf{E}-\mathbf{E}\times\mathbf{\Delta}^{(\pm)})\} - \frac{ig^2}{8M^3}\boldsymbol{\sigma}\cdot\mathbf{E}\times\mathbf{E}\,. \tag{77}$$

Here $\mathbf{E}$ and $\mathbf{B}$ are defined in terms of the cloverleaf field, Eqs. (49) and (64),

$$E^i(x) = F_{0i}^{(c)}(x), \tag{78}$$

$$B^i(x) = \tfrac{1}{2}\epsilon_{ijk}F_{jk}^{(c)}(x)\,. \tag{79}$$

The difference operators in these terms act on all the fields, $\mathbf{E}$, $\mathbf{B}$, and $G(\mathbf{x},t)$, to their right. However, the $\mathbf{D}\cdot\mathbf{E}-\mathbf{E}\cdot\mathbf{D}$ operator may be simplified since the net effect is to differentiate only the $\mathbf{E}$ field. Using Eq. (51), it can be written as

$$\mathbf{\Delta}^{(\pm)}\cdot\mathbf{E} = \frac{1}{2a}\sum_i\left[U_{x,i}E^i(x+a\hat{\imath})U_{x,i}^\dagger - U_{x-a\hat{\imath},i}^\dagger E^i(x-a\hat{\imath})U_{x-a\hat{\imath},i}\right]. \tag{80}$$

Finite lattice spacing corrections are included in δH_{spin} by using $\tilde{\mathbf{E}}$ and $\tilde{\mathbf{B}}$ of Eq. (64) and $\tilde{\mathbf{\Delta}}^{(\pm)}$ of Eq. (57) in place of $\mathbf{E}$, $\mathbf{B}$, and $\mathbf{\Delta}^{(\pm)}$. These are unnecessary in the other operators, which are already sufficiently accurate.

Certain correction terms may be unimportant in some calculations. The $O(v^2)$ corrections for spin-independent quantities are all included in $\delta H_{K,v^2}$, δH_{v^2}, and δH_{spin}; the term $\delta H_{\mathrm{spin},v^2}$ enters only at order v^4. Spin splittings, however, are themselves $O(v^2)$, and so a comparably accurate measurement of such a splitting would require all of the corrections. For simulations of light-heavy mesons, such as B's or D's, probably only the magnetic part of δH_{spin} is important. All other terms are suppressed by at least an additional power of the heavy quark velocity.

For reasons of efficiency we have separated the rela-

tivistic corrections δH from the leading-order kinetic energy $\tilde{H}_0$ in Eq. (72). This is possible because terms proportional to $\mathbf{E}$ or $\mathbf{B}$ do not cause instabilities at high momenta; it is only the kinetic terms that cause problems. The relativistic correction to the kinetic energy $\delta H_{K,v^2}$ is a special case. It probably should not be included in the evolution equation at all, but rather its contribution computed in first-order perturbation theory. The problem with this term is that it is negative and large for large momenta, eventually overwhelming the leading kinetic term $\tilde{H}_0$ and destabilizing the theory. This problem is not particular to the lattice version of NRQCD: it is a complication due to the nonrenormalizability of the theory. In fact, the continuum Hamiltonian

$$H = \frac{(\mathbf{p}+g\mathbf{A})^2}{2M} - \frac{(\mathbf{p}+g\mathbf{A})^4}{8M^3} \tag{81}$$

is not bounded below and will lead to problems if $\mathbf{p}$ is allowed to become too large. This problem does not arise in first-order perturbation theory, so that a perturbative analysis of this correction is possible. Note also that in Coulomb gauge the correction can be approximated by $-\mathbf{p}^4/8M^3$. Since this is independent of the gauge field, its perturbative contribution to mass splittings can be reliably determined given only the quark wave functions, and these are easily computed in a simulation. Alternatively, one could spread $\mathbf{\Delta}^{(2)}$ for this term over, say, five lattice spacings in each direction instead of three. This would reduce the largest effective momentum by a factor of 2, thereby reducing the high-momentum value of $\delta H_{K,v^2}$ by a factor of 16 while leaving the low-momentum behavior largely unchanged.

Many of the same problems could arise from the finite lattice spacing corrections in $\tilde{H}_0$. However, it seems that these do not cause problems for relevant values of Ma. Indeed these terms seem likely to reduce the maximum value of H_0.

A more radical way of dealing with instabilities at high momenta might be to choose Coulomb gauge, where the vector potential is small, and then replace

$$\left(1 - \frac{aH_0}{2n}\right)^n \to \exp\left[-\frac{a}{2}\left(\sqrt{\mathbf{p}^2+M^2} - M\right)\right] \tag{82}$$

in the evolution equation. Here $\mathbf{p}^2$ is the quark momentum, which is easily introduced into the simulation through the use of fast Fourier transforms. In this way the exact relativistic energy is incorporated into the simulation in a way that avoids instabilities. Unfortunately this approach greatly complicates the perturbative analysis of the theory, not least because it breaks gauge invariance. Nevertheless such problems are probably not insurmountable, and the approach may someday be useful.

Finally, note that four-fermion interactions as in Eq. (25) may be incorporated naturally into the evolution equation by replacing them with new ones which are quadratic in fermion fields. This is accomplished by introducing an auxiliary field η, a complex matrix field which is 2×2 in spin and 3×3 in color indices. For example, if η appears in the Lagrangian as

$$\mathcal{L}_\eta = a\,\psi^\dagger\eta\psi + b\,\chi^\dagger\eta^\dagger\chi + c\,\mathrm{Tr}\,\eta^\dagger\eta \tag{83}$$

without a kinetic term, this is equivalent to the interaction

$$\mathcal{L}_{\mathrm{contact}} = -\frac{ab}{c}\,\psi^\dagger\chi\chi^\dagger\psi \tag{84}$$

for the fermions. This may be seen by performing explicitly the Gaussian path integral over η, or from the equations of motion

$$\eta = -\frac{b}{c}\,\chi\chi^\dagger, \quad \eta^\dagger = -\frac{a}{c}\,\psi\psi^\dagger\,. \tag{85}$$

In a simulation this amounts to generating and summing over a random Gaussian distribution for η at each $\mathbf{x}$ and t, normalized such that

$$\langle\eta_{ij}\eta_{kl}\rangle = 0, \quad \langle\eta_{ij}\eta^*_{kl}\rangle = \delta_{ik}\delta_{jl}\,, \tag{86}$$

and propagating the quark in this field according to the interactions in $\mathcal{L}_\eta$.

V. RADIATIVE CORRECTIONS

In previous sections we derived tree-level values for the couplings of NRQCD. The couplings are modified by radiative corrections that are dominated by momenta of order π/a or larger. Since π/a is typically several GeV in simulations, we should be able to compute these radiative corrections using weak-coupling perturbation theory. However, lattice perturbation theory is notorious for its poor convergence, which is much worse than continuum QCD at comparable momenta. The large corrections, which come from tadpole and related diagrams and spoil lattice perturbation theory, apparently result from the nonlinear connection between lattice link variables and the continuum gauge potential. In the worst cases such tadpole corrections are almost as large as tree-level contributions, and some sort of nonperturbative treatment becomes necessary. Fortunately, tadpole contributions are well described by a mean-field approximation [8]. Such an approach allows us to compute most of a radiative correction nonperturbatively in terms of quantities that are easily measured in simulations. In this section we first outline a mean-field analysis for lowest-order NRQCD, giving estimates for all renormalization effects in that theory. We also compare the mean-field theory results with exact results to first order in perturbation theory. Next we discuss a simple modification of lattice NRQCD that effectively removes all tadpole contributions. Finally we comment briefly on the significance of nonperturbative contributions to the couplings.

A. Mean-field theory and lowest-order NRQCD

A simple way of tracing the effects of tadpoles is to replace the link operators $U_{x,\mu}$ in the NRQCD propagator by a number u_0 representing the vacuum expectation value of $U_{x,\mu}$. One gauge-invariant definition of u_0 is in terms of the plaquette operator

$$u_0 = \langle 0| \tfrac{1}{3}\mathrm{Tr}\, U_{\mathrm{plaq}} |0\rangle^{1/4}, \tag{87}$$

which becomes perturbatively

$$u_0 = 1 - 0.083g^2 - \cdots . \tag{88}$$

Other definitions are possible, but these give similar results and will not be considered here. With this definition, u_0 is easily measured in a simulation: for example, $u_0 = 1 - 0.122$ at $\beta = 6$. The measured u_0 includes tadpoles to all orders of perturbation theory, and perhaps also some nonperturbative effects.

Having a mean value for $U_{x,\mu}$, we may proceed with a mean-field analysis of the NRQCD propagator. In this approximation, the kinetic-energy operator is

$$H_0 \approx -\frac{1}{2Ma^2}\sum_i \left[u_0 e^{a\partial_i} + u_0 e^{-a\partial_i} - 2\right], \tag{89}$$

so that

$$H_0 \approx h_0 + u_0\frac{\mathbf{p}^2}{2M} \tag{90}$$

for a quark with a low momentum $\mathbf{p}$, where

$$h_0 = 3\left(1 - u_0\right)/Ma^2 . \tag{91}$$

Substituing this into Eq. (54) for the Green's function and replacing the link variables by u_0's, we obtain finally a mean-field approximation to the quark propagator

$$G^{\mathrm{MF}}(\mathbf{p},t) \approx u_0^{t/a}\left(1 - \frac{ah_0}{2n} - \frac{au_0}{2n}\frac{\mathbf{p}^2}{2M}\right)^{2nt/a} . \tag{92}$$

In the low-momentum limit, we expect the continuum propagator to have the form

$$G^{\mathrm{cont}}(\mathbf{p},t) = Z_\psi^{\mathrm{MF}} \exp\left[-t\left(E_0^{\mathrm{MF}} + \frac{\mathbf{p}^2}{2Z_M^{\mathrm{MF}}M}\right)\right] . \tag{93}$$

Matching these, we obtain

$$E_0^{\mathrm{MF}} = -a^{-1}\ln\left[u_0\left(1 - ah_0/2n\right)^{2n}\right] \tag{94}$$

for the zero-point energy induced by tadpoles,

$$Z_M^{\mathrm{MF}} = u_0^{-1}\left(1 - ah_0/2n\right) \tag{95}$$

for the mass renormalization, and

$$Z_\psi^{\mathrm{MF}} = 1 \tag{96}$$

for the quark field renormalization. At $\beta = 6$ with $Ma = 2$ (roughly the b quark mass) and $n = 1$, these renormalization parameters are

$$\begin{aligned} E_0^{\mathrm{MF}} &\approx 0.9\ \mathrm{GeV}, \\ Z_M^{\mathrm{MF}} &\approx 1.04, \\ Z_\psi^{\mathrm{MF}} &= 1. \end{aligned} \tag{97}$$

None of the renormalizations is particularly large for leading-order NRQCD, at least for β near 6. This is despite the theory's nonrenormalizability and consequent power-law divergent renormalizations: for example, $ah_0 \propto 1/a$. These divergences cause problems as the lattice spacing a is reduced, but there will be little need to reduce a once our finite-a corrections have been incorporated.

Renormalization parameters such as E_0, Z_M, and Z_ψ are needed to interpret simulation results. For example, the total mass of a meson with NRQCD energy E_n is

$$M_n = 2\left(Z_M M - E_0\right) + E_n . \tag{98}$$

Knowing Z_M and E_0 from mean-field theory, perturbation theory, or both, and E_n from simulations, we can use this expression to tune the NRQCD bare quark mass. The wave-function renormalization is important when designing quark operators to describe such things as radiative transitions or decays through quark annihilation. For example, the continuum operator $\chi^\dagger\psi$, describing quark-antiquark annihilation, is well modeled by the lattice operator $\chi^\dagger\psi/Z_\psi$.

We can calibrate the reliability of mean-field theory by comparing mean-field results with exact calculations to first order in perturbation theory. Such calculations have been performed by Davies and Thacker [3], who have analyzed the NRQCD propagator through one-loop order. They defined the propagator by means of the evolution equation

$$\begin{aligned} G(\mathbf{x},t+a) &= U_{x,t}^\dagger\left(1 - \frac{a\,H_0}{n}\right)^n G(\mathbf{x},t) + U_{x,t}^\dagger\,\delta_{x,0}\,\delta_{t,0}, \\ G(\mathbf{x},t) &= 0 \quad (t \le 0), \end{aligned} \tag{99}$$

which differs slightly from our equation. The energy shift and mass renormalization for this equation are identical to ours if n is replaced by $n/2$ in our equations. The wave-function renormalization, however, is significantly different: in mean-field theory, one finds $Z_\psi^{\mathrm{MF}} = (1 - ah_0/n)^{-n}$ for the Davies-Thacker equation. In Table II we list the $O(g^2)$ coefficients for E_0, Z_M, and Z_ψ. We give both the exact result, as computed by Davies and Thacker using perturbation theory, and the mean-field estimate, obtained by replacing u_0 with its perturbative expansion, Eq. (88), in mean-field expressions for the renormalization parameters. Since we expect nontadpole contributions of one or two times α_s/π, or $0.03g^2$ to $0.05g^2$, the agreement is excellent. A nontadpole contribution of this size is only 5–10 % of the tree-level contribution at $\beta = 6$. Mean-field theory does seem to account well for radiative corrections when they are large.

When perturbative results are known, they can be used to correct the mean-field prediction. For example, the zero-point energy E_0 for our propagator at $aM = 1.5$ can be written as

$$aE_0 = -\ln\left[u_0\left(1 - ah_0/2\right)^2\right] + 0.07\,\frac{g^2}{u_0^4} . \tag{100}$$

The correction $0.07g^2$ is the difference between the perturbative and mean-field result in Table II. The factor $1/u_0^4$ in the correction accounts for tadpole-induced renormalization of the bare coupling $g^2 = 6/\beta$, also suggested by mean-field theory [8]. With this expression, all

TABLE II. The coefficient of g^2 in expansions of the NRQCD renormalization parameters. Results coming from exact perturbation theory (PT) are compared with estimates based on mean-field theory (MFT) for a variety of masses M. The parameters are appropriate to the evolution equation used by Davies and Thacker. For Z_M, $n = 1$ for $Ma = \infty$ and 5; $n = 2$ for $Ma = 2.5$ and 1.5. E_0 and Z_ψ are independent of n. An infrared divergence, which is shared with the continuum theory, has been omitted from Z_ψ.

Ma	PT	MFT
	aE_0/g^2	
∞	0.17	0.08
5	0.21	0.14
2.5	0.25	0.18
1.5	0.30	0.23
	$(Z_M - 1)/g^2$	
∞	0.07	0.08
5	0.04	0.03
2.5	0.07	0.03
1.5	0.06	0.0
	$(Z_\psi - 1)/g^2$	
∞	0.04	0
5	0.07	0.05
2.5	0.10	0.10
1.5	0.15	0.17

that is needed to complete the calculation is a measurement of the expectation value of the trace of the plaquette to determine u_0.

B. Removing tadpole contributions

Our mean-field analysis of lowest-order NRQCD is readily extended to include the various corrections due to relativity and finite lattice spacing. There is, however, a simpler way of dealing with the tadpoles. By dividing every link matrix by u_0 before computing quark propagators, all tadpole contributions are automatically removed from the simulation. When we replace $U_{x,\mu}$ with $U_{x,\mu}/u_0$ in our formulas, we are in effect redefining the coupling constants [at $O(\alpha_s)$]. Perturbation theory should be quite convergent for these new couplings, and, in particular, the tree-level results we have computed should be accurate to within corrections of order α_s/π; that is, to 5–10 % at $\beta = 6.0$.

The mean-field corrections introduced by our simple procedure are not always small, particularly for operators that involve the cloverleaf definitions of electric or magnetic fields. These operators are modified by a factor u_0^{-4}: for example, $\mathbf{B} \to \mathbf{B}/u_0^4$. At $\beta = 6.0$, u_0^{-4} is 1.7, almost doubling the $\mathbf{E}$ and $\mathbf{B}$ fields. Leaving out such factors leads to dramatic underestimates of quantities, such as spin splittings, that involve one or more powers of $\mathbf{E}$ or $\mathbf{B}$.

C. Nonperturbative effects

As is true of all perturbative calculations, our analysis of NRQCD couplings omits nonperturbative contributions. *A priori*, we know little about the nature of such contributions. The one thing we may assert with some confidence is that nonperturbative contributions are smaller than perturbative contributions for momenta π/a larger than a couple of GeV; that is, for $\beta > 5.7$. This is the fundamental assumption underlying all applications of perturbative QCD, whether in the continuum or on the lattice. As we have argued, perturbative corrections to our couplings are probably less than 10–15 % for reasonable β's, and so it seems likely that nonperturbative effects are no larger than a few percent. Since most physical results are not extremely sensitive to the values of the couplings, the nonperturbative effects are probably safely neglected.

Our mean-field analysis supports this view by providing a toy model for nonperturbative effects. The plaquette operator plays a key role in this analysis since it determines the mean field u_0. The plaquette is one of the few operators whose nonperturbative behavior is somewhat understood. The expectation value of a large Wilson loop with area A contains a factor $\exp(-\sigma A)$ due to nonperturbative confinement. Here σ is about 0.18 GeV^2, based upon phenomenologically motivated quark-antiquark potentials. There is empirical evidence that this behavior persists for small loops, and even for the plaquette, whose expectation value seems well described by perturbation theory times a factor of $(1-\sigma a^2)$, at least for β near 6.0 [8]. At $\beta = 6.0$, σa^2 is about 0.04, making the nonperturbative part of the plaquette about 10% of the size of the $O(g^2)$ part. This is perhaps some indication of the relative sizes of perturbative and nonperturbative effects.

To continue with our toy model, we assume that the mean-field parameter u_0 inherits a nonperturbative contribution $-\sigma a^2/4$ from the plaquette:

$$u_0^{\text{toy}} = u_0^{\text{pert}} - \sigma a^2/4 . \tag{101}$$

This amounts to less than 2% of u_0^{toy} at $\beta = 6.0$, and less at higher β's, so it has a negligible effect on renormalization constants like Z_M and Z_ψ. One place where one might worry about nonperturbative corrections is in the very divergent zero-point energy,

$$\begin{aligned} E_0 &\approx (1 - u_0)\left(1/a + 3/Ma^2\right) \\ &\to E_0^{\text{pert}} + \sigma a/4 + 3\sigma/4M . \end{aligned} \tag{102}$$

Here there is a contribution that does not vanish with a; factors of $1/a$ generated by perturbative power-law divergent loops cancel the factors of a in the nonperturbative term. However, this contribution amounts to only about 30 MeV for b quarks, much less than the perturbative contribution of about 900 MeV at $\beta = 6$.

Nonperturbative terms such as those in Eq. (102) for E_0 mean that the perturbative relation, Eq. (98), between quark mass and meson mass cannot be exact for any lattice spacing. But for $\beta = 6.0$, the uncertainty that results is only a few percent of the b quark mass. Of course, ours is only a toy model for nonperturbative effects. We do not really know that the nonperturbative part of u_0 is suppressed by a^2 rather than, say, a^4 or

$a^{1/2}$. But we do know that it is suppressed relative to the $O(g^2)$ contributions. Thus we can use perturbative results to bound nonperturbative contributions; as long as perturbative corrections are not individually large, nonperturbative corrections cannot be very important. In some cases, the use of the measured value of u_0, rather than the calculated one, may account for some of the nonperturbative physics. This is most likely the case, for example, when renormalizing cloverleaf $\mathbf{E}$'s and $\mathbf{B}$'s with the plaquette average.

Finally it is worth noting that the nonperturbative contribution to the plaquette expectation value is almost comparable in magnitude to the $O(g^4)$ perturbative contribution at $\beta = 6.0$. Thus there seems little point in computing much beyond first or second order in g^2. Precision beyond a few percent will probably require nonperturbative tuning of couplings.

VI. CONCLUSIONS

Nonrelativistic QCD provides one of the most efficient frameworks for simulating heavy quarks. While an approximation to QCD, it may be systematically improved; this paper provides initial steps toward that goal. We developed general power-counting rules which allowed us to assess the relative importance of various corrections, and which we can use to fine-tune the theory for specific applications. We computed all of the leading-order corrections required by relativity, both for spin-independent and spin-dependent interactions. The theory was then adapted to the lattice, including all leading-order corrections from finite lattice spacing. Finally, we presented a simple mean-field procedure that automatically incorporates the largest radiative corrections to the NRQCD coupling constants. Our mean-field analysis also allowed us to estimate the importance of nonperturbative contributions to the couplings.

In NRQCD, heavy-quark propagators are determined by a simple evolution equation, avoiding the need for costly matrix inversion. Our fully corrected evolution equation was presented in Sec. IV C. Using this equation, together with the mean-field improvement procedure described in Sec. V, should give results for ψ and Υ mesons that are accurate to perhaps 10% or better, depending upon the measurement. The largest remaining errors are probably due to uncalculated $O(\alpha_s)$ corrections to the NRQCD couplings beyond the mean-field contributions, and to light-quark vacuum polarization. These errors can be removed in the near future. The coupling constant corrections are computed using ordinary one-loop weak-coupling perturbation theory; work has already begun on these. The dominant contribution from light-quark vacuum polarization is probably insensitive to light-quark masses less than 100–200 MeV, and the extrapolation to realistic quark masses should be quite smooth. It is therefore feasible to include the light quarks with current lattice technology. Once these systematic effects have been removed, simulations should be accurate to a few percent, where nonperturbative contributions to the couplings may become important.

Simulations using the techniques presented in this paper should, in the near future, produce accurate spectra, decay rates, wave functions, and other matrix elements for all of the lowest-lying mesons in the ψ and Υ families. These techniques should also be useful in studies of D and B, as NRQCD propagators are more efficiently generated than relativistic propagators, and much less afflicted by noise than static propagators [8]. With these methods we are entering a new era of high-precision lattice simulations of quantum chromodynamics.

ACKNOWLEDGMENTS

We are grateful to C. Davies, I. Drummond, R. Horgan, P. Mackenzie, and B. Thacker for discussions, comments, and suggestions. This work was supported in part by a grant from the National Science Foundation. K.H. was supported in part by the Department of Energy and by Ohio State University. U.M. was supported by the Academy of Finland, and would like to thank Cornell University for hospitality during the completion of this work.

APPENDIX

This appendix discusses the construction in NRQCD of lattice operators which reproduce the corresponding continuum operators to any desired order in a, at tree level. We first describe a natural technique which works for all bilinears in fermion fields, but turns out to be inconvenient in actual simulations. Then we show how to circumvent this problem by starting with a convenient lattice operator and computing corrections to it. Finally, we discuss in some detail the corrections to the gluon action in the non-Abelian case.

Consider a general local, gauge-covariant, continuum operator, bilinear in the fermion fields and with canonical dimension $d = n + 3$:

$$O(x) = \psi^\dagger(x) K_n(\mathbf{E}, \mathbf{B}, \mathbf{D}, D_t)\psi(x) . \tag{A1}$$

Since the field strength components are proportional to commutators of covariant derivatives, such an operator is a linear combination of the tensors

$$O_{\mu_1,\ldots,\mu_n}(x) \equiv \psi^\dagger(x) D_{\mu_1} \cdots D_{\mu_n}\psi(x) . \tag{A2}$$

It is straightforward to construct lattice expressions for these tensors, accurate to a specific order in a, provided one defines the link variables correctly in terms of the continuum gauge potentials, as in Eq. (55). The relationship between the continuum covariant derivatives and the corresponding finite differences on the lattice is then given by Eq. (56), and one can rewrite the tensors in Eq. (A2) using, for example, the symmetric expression

$$D_\mu = \frac{1}{2a}\left[\ln(1 + a\Delta_\mu^{(+)}) - \ln(1 - a\Delta_\mu^{(-)})\right] . \tag{A3}$$

In practice of course one always works with the first few terms in the power series expansion of Eq. (A3). One

can then use the fact that $\Delta_\mu^{(+)} = \Delta_\mu^{(-)} + O(a)$ to construct an expression for D_μ that is maximally local on the lattice, as for example Eq. (57). To see what kind of lattice expressions are generated through this procedure, consider, for example,

$$O_{[\mu\nu]}(x) \equiv -ig\,\psi^\dagger(x)F_{\mu\nu}(x)\psi(x)\,. \tag{A4}$$

Using Eq. (57), this becomes, up to corrections $O(a^4)$,

$$O_{[\mu\nu]}(x) = \psi^\dagger(x)\left[\left(\Delta_\mu^{(\pm)}\Delta_\nu^{(\pm)} - \frac{a^2}{6}\Delta_\mu^{(\pm)}\Delta_\nu^{(+)}\Delta_\nu^{(\pm)}\Delta_\nu^{(-)} - \frac{a^2}{6}\Delta_\mu^{(+)}\Delta_\mu^{(\pm)}\Delta_\mu^{(-)}\Delta_\nu^{(\pm)}\right) - (\mu \Leftrightarrow \nu)\right]\psi(x)\,. \tag{A5}$$

In terms of link variables the result is simpler and more transparent, and it is shown in Fig. 2. There one can see the main characteristic common to all lattice operators constructed this way: the quark field and its hermitian conjugate are evaluated at different points on the lattice. In actual simulations, this turns out to be a serious disadvantage: it is much more economical to define both fermions at the same site.

Fortunately, it is as easy to go from a lattice operator written in terms of link variables to the corresponding continuum expression. We can therefore start with any operator having the appropriate continuum limit, such as our cloverleaf $F_{\mu\nu}^{(c)}(x)$, and then correct it to the desired order in a. Consider for example the first term in the cloverleaf definition of the field strength tensor, sandwiched between spinors:

$$\psi^\dagger(x)U_{x,\mu}U_{x+a\hat{\mu},\nu}U^\dagger_{x+a\hat{\nu},\mu}U^\dagger_{x,\nu}\psi(x)\,. \tag{A6}$$

It is easy to find an expression written in terms of lattice derivatives that will reproduce this term. One starts by replacing each matrix U_μ with a forward derivative $\Delta_\mu^{(+)}$, and each matrix $U_\mu^\dagger$ with the corresponding backward derivative. This gives

$$\psi^\dagger(x)\Delta_\mu^{(+)}\Delta_\nu^{(+)}\Delta_\mu^{(-)}\Delta_\nu^{(-)}\psi(x)\,, \tag{A7}$$

which contains Eq. (A6), plus correction terms with at most three U's, that are easily calculated. The procedure is then iterated until all terms with a lower number of U's are canceled. Once the desired lattice operator is written in terms of lattice derivatives, the corresponding continuum operator can be calculated using, once again, Eq. (56), to the desired order in a.

This procedure identifies the terms which need to be subtracted from the original definition. Once known in the continuum, it is easy to guess a lattice expression that will cancel them, yielding the corrected lattice operator. The result for the cloverleaf field strength is, as expected, given by Eq. (63) and Eq. (64).

The correction to the gluon action in the non-Abelian theory is somewhat more complicated to check directly. We start by noting that, to all orders in a, the link variable can be written as

$$U_{x,\mu} = \exp\left[\sum_{n=1}^{\infty}\left(a^n u^b_{n,\mu}T_b\right)\right]\,. \tag{A8}$$

This is a consequence of the Baker-Campbell-Hausdorff theorem, that allows us to rewrite the path-ordered exponential as exponential of a series of commutators. Our definition of the link variable, with the gauge potentials evaluated at midlink, implies, for example,

$$\begin{aligned} u^b_{1,\mu} &= -igA^b_\mu, \\ u^b_{2,\mu} &= u^b_{4,\mu} = 0, \\ u^b_{3,\mu} &= -i\frac{g}{24}\partial^2_\mu A^b_\mu - i\frac{g^2}{12}f_{bcd}A^c_\mu\partial_\mu A^d_\mu\,, \end{aligned} \tag{A9}$$

where f_{bcd} are the structure constants of SU(3). By the same token, we can write the plaquette matrix as

$$U_{P(x,\mu\nu)} = \exp\left[\sum_{n=1}^{\infty}\left(a^n C^b_{n,\mu\nu}T_b\right)\right]\,, \tag{A10}$$

where, with the fields at the center, one easily finds that

$$C^b_{1,\mu\nu} = 0, \quad C^b_{2,\mu\nu} = -igF^b_{\mu\nu}\,. \tag{A11}$$

The series expansion in powers of a of the trace of Eq. (A10) can be considerably simplified by using the trace identities

$$\begin{aligned} &\mathrm{Tr}(T_a) = 0, \quad \mathrm{Tr}(T_aT_b) = \tfrac{1}{2}\delta_{ab}, \\ &\mathrm{Tr}(T_aT_bT_c) = \tfrac{1}{4}(d_{abc} + if_{abc})\,, \end{aligned} \tag{A12}$$

where d_{abc} is the completely symmetric invariant tensor of SU(3). This yields

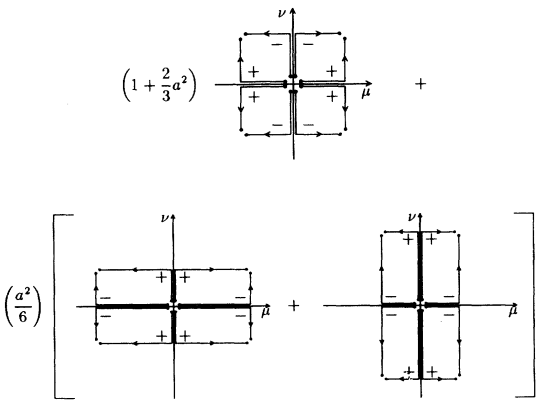

FIG. 2. The operator $-ig\psi^\dagger(x)F_{\mu\nu}\psi(x)$, corrected to order a^4. The sign that each term bears in the sum appears at the corner of the corresponding Wilson line. The field $\psi^\dagger$ is at the beginning of each line, the field ψ at the end.

$$\mathrm{Tr}(U_{P(x,\mu\nu)}-1)=\frac{a^4}{4}\mathbf{C}_{2,\mu\nu}\cdot\mathbf{C}_{2,\mu\nu}+\frac{a^5}{2}\mathbf{C}_{2,\mu\nu}\cdot\mathbf{C}_{3,\mu\nu}+\frac{a^6}{2}\mathbf{C}_{2,\mu\nu}\cdot\mathbf{C}_{4,\mu\nu}+\frac{a^6}{4}\mathbf{C}_{3,\mu\nu}\cdot\mathbf{C}_{3,\mu\nu}+\frac{a^6}{24}C^a_{2,\mu\nu}C^b_{2,\mu\nu}C^c_{2,\mu\nu}d_{abc}+O(a^7)\,, \tag{A13}$$

so that the only coefficients we need to calculate are $\mathbf{C}_{3,\mu\nu}$ and $\mathbf{C}_{4,\mu\nu}$. The calculation is rather lengthy, but can be performed using a symbolic manipulation program, such as MATHEMATICA [9]. The result is

$$C^a_{3,\mu\nu}T_a=-\frac{g^2}{2}\left[A_\mu+A_\nu,F_{\mu\nu}\right], \tag{A14}$$

$$C^a_{4,\mu\nu}T_a=-\frac{ig}{24}(D^2_\mu+D^2_\nu)F_{\mu\nu}+\frac{g^2}{8}\left[(\partial_\mu+\partial_\nu)(A_\mu+A_\nu),F_{\mu\nu}\right]+\frac{ig^3}{8}\left[A_\mu+A_\nu,[A_\mu+A_\nu,F_{\mu\nu}]\right].$$

Substituting Eq. (A11) and Eq. (A14) in Eq. (A13) one can verify, as a nontrivial check, that all gauge-noninvariant terms disappear, as do the coefficients of odd powers of a. The final result is, as expected,

$$\mathrm{Tr}\left[R\left(U_{P(x,\mu\nu)}\right)\right]=-\frac{g^2a^4}{2}\mathrm{Tr}(F^2_{\mu\nu})-\frac{g^2a^6}{24}\mathrm{Tr}\left[F_{\mu\nu}(D^2_\mu+D^2_\nu)F_{\mu\nu}\right], \tag{A15}$$

the non-Abelian generalization of Eq. (66).

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