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Heavy-quark renormalization parameters in nonrelativistic QCD

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We calculate the self-energy of the heavy quark to $O(\alpha_s)$ in nonrelativistic QCD (NRQCD) on the lattice. We use the lowest-order (in $1/M$) NRQCD action which includes the time derivative and kinetic energy terms, but we ignore spin effects. Results are given for the wave-function renormalization, mass renormalization, and energy shift. Our results agree with the lowest-order static effective field theory as $Ma \to \infty$, where Ma is the quark mass in lattice units. At values of Ma appropriate to b- and c-quark calculations, the differences are significant. We also consider $1/Ma$ corrections to the static theory arising from the kinetic term.

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I. INTRODUCTION

Recently the first nonperturbative calculations involving dynamical heavy quarks on a lattice have demonstrated that it will soon be possible to extract quantitative information on heavy-quark bound states [1]. These calculations make use of an effective field theory, nonrelativistic QCD (NRQCD), which is suited to the physics and numerical simulation of heavy-quark systems. Given the experimental data now available, it is clear that calculations using NRQCD on the lattice can provide a precise nonperturbative test of QCD with a fraction of the computing resources required for light-quark physics.

To achieve this precision requires systematically extending the set of operators used in the Lagrangian of NRQCD and tuning their coupling constants. Since the choice of coupling constants is in principle a perturbative problem, a whole series of calculations in lattice perturbation theory must be performed if this program is to be realized. In this paper we present the first of these calculations.

To simulate in detail the physics of energy scales up to and beyond the heavy-quark mass M is a difficult task in lattice QCD and largely a waste of computer time. The energy scale M is not important for the low-energy physics of heavy-quark bound states and is well separated from the much smaller scales of quark momentum and kinetic energy which are important. In NRQCD we therefore exclude momenta above the scale M by imposing a cutoff Λ of order M. We can then concentrate computing power on the important low-energy scales.

A useful Lagrangian for NRQCD is obtained by expanding the usual relativistic quark Lagrangian in powers of the inverse quark mass. The lowest-order spin-independent terms consist of a single time derivative and a nonrelativistic kinetic energy term. This Lagrangian has been successfully used for a preliminary study of the Υ and Ψ systems [1]. Spin-dependent terms start at $1/M$ with a coupling to the gluon chromomagnetic field. Higher-dimension operators can then be added, suppressed by additional powers of $1/M$ or by the lattice spacing a.

For a given calculation and required accuracy, a decision can be made as to how many operators to include in the Lagrangian. The coupling constants of these operators must also be known with sufficient accuracy and this requires adjusting them from their value at the tree level given by the $1/M$ expansion. The coupling constants must account for the effect of loop diagrams with highly ultraviolet momenta ($> \Lambda$) which are present in QCD but not in NRQCD. Their effect is the same as that of having the local operators already present in NRQCD but with a coefficient which is a power series in $g^2(\Lambda)$. We can therefore mimic it by setting the coupling constants of NRQCD to be the appropriate power series required to match full QCD. If Λ is large enough, $g^2(\Lambda)$ is a small expansion parameter and we can sensibly demand a certain level of accuracy in g^2.

The coupling constants that result, however, will generally contain powers of Λ/M and so diverge as Λ/M becomes large, even as $g^2(\Lambda)$ becomes small. This simply reflects the breakdown of perturbation theory for the effective theory in that limit. We might expect perturbation theory to be accurate in the region around $\Lambda \sim M$ for large M. The size of this region will depend on the numerical size of the coefficients of the divergent terms and can only be decided by doing the perturbative calculation. The alternative is to tune the couplings numerically to fit experiment and this will certainly increase the complexity of the numerical calculation. Also, if the coupling constants can be fixed perturbatively, the theory will have its maximum predictive power.

We must always give up some predictions, however, to fix certain parameters of the theory. In light-quark physics we must fix the lattice spacing and quark mass in this way. For heavy-quark physics with NRQCD we have these two parameters and an additional one—the zero point of energy. When the Lagrangian of NRQCD

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is defined an energy shift is performed to remove the usual mass term at the tree level. As we shall see in this paper, loop diagrams generate an energy shift term with a coefficient proportional to Λ, since no symmetry prevents it. In principle, the energy shift can be determined in perturbation theory, like the other coupling constants. This would then allow a numerical simulation to predict absolute energies. Whether this is feasible depends upon the value obtained.

In this paper we present results for the $O(\alpha_s)$ corrections to the heavy-quark self-energy in NRQCD calculated in lattice perturbation theory. We work with the lowest-order (in $1/M$) NRQCD Lagrangian with no spin effects included. We obtain the wave-function renormalization, mass renormalization, and energy shift required to match full continuum QCD. We give results for an infinite-volume lattice for different values of the quark mass in lattice units, Ma. We also give results for finite spatial lattice volume.

In addition, we compare NRQCD to the static effective theory [2], which retains only the time derivative part of the action and treats the kinetic term as a perturbation. The static effective theory has been used to simulate bound states of heavy quarks with light quarks [3]. It is not appropriate for the bound states of purely heavy quarks. The expansion in powers of $1/M$ is organized differently in the static theory and this gives rise to different coupling constants beyond the tree level.

The plan of the paper is as follows. In Sec. II we present our action and Feynman rules. Section III contains the $O(\alpha_s)$ corrections to the heavy quark self energy. In Sec. IV we discuss the results and their usefulness for numerical simulations. Section V contains our conclusions.

II. NRQCD LATTICE FEYNMAN RULES

To lowest order, the nonrelativistic lattice action can be written

$$S_Q = a^3 \sum_{\mathbf{x}t} \psi^\dagger_{\mathbf{x}t} \left(\Delta_4 - \sum_{j=1}^{3} \frac{\Delta_j \Delta_{-j}}{2Ma} \right) \psi_{\mathbf{x}t} . \tag{1}$$

The gauge-covariant difference operators are defined by

$$\begin{aligned} \Delta_\mu \psi_x &= U_{x,\mu} \psi_{x+\hat{\mu}} - \psi_x \ , \\ \Delta_{-\mu} \psi_x &= \psi_x - U^\dagger_{x-\hat{\mu},\mu} \psi_{x-\hat{\mu}} \ , \end{aligned} \tag{2}$$

where $U_{x,\mu}$ is the usual lattice link variable at site $x = (\mathbf{x}, t)$ in direction μ (representing the gauge field) and $\psi_{\mathbf{x}t}$ is the quark field at spatial site $\mathbf{x}$ and time t. An energy shift has been done to remove the usual mass term [4]. Note that we have omitted all spin terms from the action even though $\boldsymbol{\sigma}\cdot\mathbf{B}/2M$ is the same order in $1/M$ as the kinetic term. It is not as important as the kinetic term for spin-independent quantities. A more complete calculation will include it [5].

The propagator satisfies the evolution equation [6]

$$G_{\mathbf{x}t+1} = U^\dagger_{\mathbf{x}t,4} [(1 - H) G_{\mathbf{x}t} + \delta_{t,0} \delta_{\mathbf{x},0}] \ , \tag{3}$$

$$G_{\mathbf{x}t} = 0, t \le 0 \ , \tag{4}$$

where H is the gauge-covariant operator

$$H = - \sum_j \frac{\Delta_j \Delta_{-j}}{2Ma} \ . \tag{5}$$

The NRQCD lattice Feynman rules for heavy quarks derived from Eq. (1) are given in Fig. 1. We work in the Feynman gauge and take the gluon field to sit at the center of a link. A gluon mass λ is introduced to provide an infrared cutoff.

Note that our approach is different from that of the static effective theory [2], which however uses the same action. There the kinetic energy term is treated as a perturbation, so that at every order in $1/M$ it gives rise to new contributions which are not suppressed by g. In NRQCD the kinetic energy term is included in the quark propagator. This means that contributions to the self-energy that result from the operators in Eq. (1) are automatically included completely at a fixed order in g^2. When Eq. (1) is extended to include additional terms, e.g., $\psi^\dagger (D^4/M^3) \psi$, all those with order-1 coupling constants will be included in the quark propagator. All vertices will be at least $O(g)$. We shall see the effect of this difference in the two theories later.

We want to work in a region where the lattice spacing

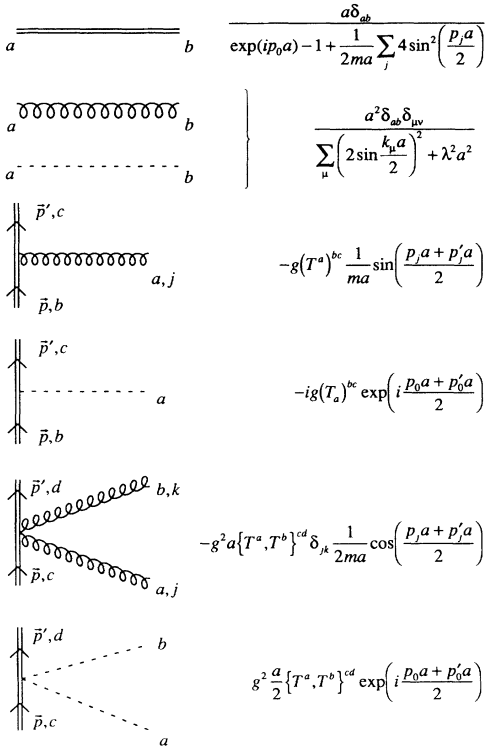

FIG. 1. Feynman rules for the action of Eq. (1). A dashed line indicates a temporal gluon A_0 and a curly line indicates a spatial gluon A_i. They must be integrated using $(1/a^3) \int_{-\pi}^{\pi} [d^4(ka)/(2\pi)^4]$ to give the self-energy in lattice units.

is small and perturbation theory is valid although Ma should not be too small. A problem arises, however, in numerical simulations with NRQCD, while Ma is still fairly large. The problem is that the high-momentum modes ($p_i a \sim \pi$) can tend to swamp the contribution of low-momentum modes when numerical precision is limited. The region where this happens can be seen by performing the Fourier transform of the free lattice quark propagator. We have

$$\int_C dz \left(\frac{z^{t-1}}{z - 1 + 4\sum_i [\sin(p_i a/2)]^2/2Ma} \right) \tag{6}$$

where $z = \exp(ip_0 a)$. In the numerical work we select forward propagation in time and we must enforce this in any analytic calculation. This means we must choose the z contour so that the pole in the propagator is inside the contour for all values of the spatial momentum. For

$$\frac{4\sum_i [\sin(p_i a/2)]^2}{2Ma} > 2 \tag{7}$$

we must distort the contour away from a unit circle. The integral then gives

$$\left(1 - \frac{4\sum_i [\sin(p_i a/2)]^2}{2Ma} \right)^{t-1} . \tag{8}$$

If $Ma < 3$ modes with high spatial momenta will satisfy Eq. (7) and will give a contribution to the quark propagator which actually grows with t. On a computer it may then be difficult to separate the small contribution of physical low-momentum modes from underneath this huge background.

This instability in the evolution equation corresponds to the well-known numerical instability of the diffusion equation if the time step is too large. The usual remedy is to take smaller time steps or, on the lattice, to reduce the temporal lattice spacing. However, in general, gluon field configurations are generated with the same lattice spacing in all directions and so another remedy is necessary. In the numerical simulations of Ref. [1] the nonrelativistic action was modified so that the evolution equation becomes

$$G_{\mathbf{x}t+1} = U^\dagger_{\mathbf{x}t,4} \left[\left(1 - \frac{1}{n} H \right)^n G_{\mathbf{x}t} + \delta_{t,0}\delta_{\mathbf{x},0} \right] , \tag{9}$$

where n is a small integer. This equation is stable for masses of order $3/n$ or larger. The modified action differs from the original action by $O(a/M)$ corrections. Clearly as $n \to \infty$ the central term of the evolution equation will look like $\exp(-H)$ which is the version appropriate for continuum time. No problem with high-momentum modes occurs in that case. For n=2 the action becomes

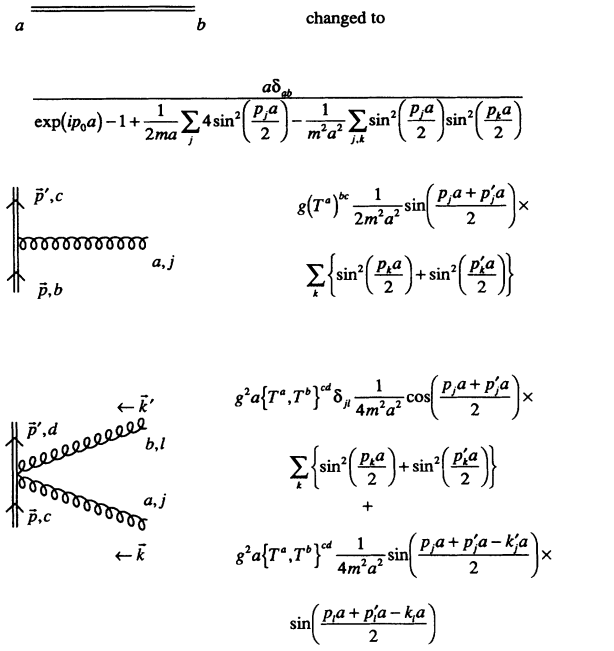

FIG. 2. Additional Feynman rules for interactions between quarks and spatial gluons, when the action of Eq. (10) is used.

$$S_Q = a^3 \sum_{\mathbf{x}t} \psi^\dagger_{\mathbf{x}t} \left(\Delta_4 + H - \frac{H^2}{4} \right) \psi_{\mathbf{x}t} \tag{10}$$

and the evolution will be stable for $Ma > 1.5$.

Since this is the action that has been used in numerical work for $Ma < 3$ [1], it is the action we use for perturbative calculations also. We quote the results for $n = 1$ and $n = 2$. The additional Feynman rules for the $n = 2$ case are given in Fig. 2.

Analytically we can always take a smaller temporal lattice spacing if we wish, and we will discuss this case also. It may turn out to be the numerical solution of choice in the future, since the computational time required is shorter. We take a temporal lattice spacing a_t and a spatial lattice spacing a with $na_t = a$. n can then be chosen appropriately to prevent instability of the high-momentum modes. No adjustment of the action is necessary. The Feynman rules for this case [7] are a simple modification of those in Fig. 1. Every occurrence of the sine of a spatial momentum is divided by n, and there is an overall factor of $1/n^3$ multiplying each Feynman diagram.

For the static theory the numerical problem with high-momentum modes on the lattice does not arise. The propagator is evolved forward in time using a variant of Eq. (3) in which the operator H is treated as a perturbation and acts only on a small number of time slices. In analytic calculations there is no kinetic energy term in the quark propagator; propagation forward in time is enforced by an ϵ prescription. As we shall see, this gives rise to another problem in which perturbative coefficients have large mass-dependent contributions.

III. ORDER-α_S CORRECTIONS TO THE HEAVY-QUARK PROPAGATOR

The diagrams which contribute to the mass and wave-function renormalization and the energy shift of the heavy quark are shown in Fig. 3. At $O(g^2)$ we write the quark self-energy in lattice units as

$$\Sigma(p) = Aa + B\frac{4}{2Ma}\sum_i \left(\sin\frac{p_i a}{2}\right)^2 + C\left[\exp(ip_0 a) - 1 + \frac{4}{2Ma}\sum_i \left(\sin\frac{p_i a}{2}\right)^2\right] + \cdots \quad (11)$$

for small values of the quark momentum $\mathbf{p}$, and energy p_0 and the action of Eq. (1). For Eq. (10) the term multiplying C is modified to include the appropriate quartic terms in the spatial momentum from the zeroth-order self-energy. We write the self-energy in this form so that it combines easily with the zeroth-order term. It is of course indistinguishable at small pa from the continuum form.

Ag^2 is then the energy shift for the quark propagator in GeV. B is the $O(g^2)$ contribution to the mass renormalization and C is part of the $O(g^2)$ contribution to the wave-function renormalization. We discuss this in more detail in Sec. IV.

The constant A is calculated by simply setting the quark momenta and energy to zero on the external legs of all the diagrams. B is found by setting the quark on shell $\{\exp(ip_0a) - 1 + 4[\sin(pa/2)]^2/2Ma\}=0$ for $n=1$, taking the second derivative with respect to the three-momentum $\mathbf{p}a$, and then setting $\mathbf{p}a$ to zero. C is calculated by setting $\mathbf{p}a$ to zero, taking the derivative with respect to the energy p_0a, and then setting p_0a to zero. The integrals over loop momenta (k) must be done numerically; we used VEGAS [8] to evaluate them. Note that the integrals are a function of the product Ma only and not M or a separately.

One useful numerical check is that in the $Ma \to \infty$ limit we should agree with the results of the static effective theory to zeroth order in $1/M$ at $O(g^2)$ [2]. This follows simply by looking at the integrals and noticing that in that limit the terms containing spatial quark momenta are always small and can be neglected. An appropriate ϵ prescription must be chosen instead, to enforce forward propagation in time. The integrals then become those of the static theory.

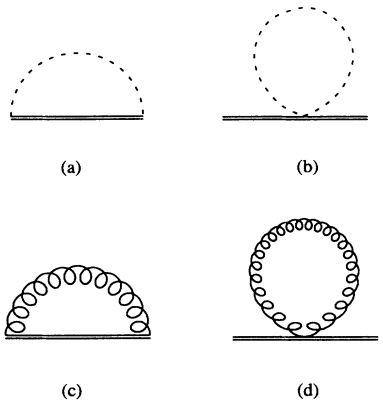

FIG. 3. Diagrams which contribute to the heavy-quark self-energy. A dashed line indicates a temporal gluon A_0. A curly line indicates a spatial gluon A_i.

Beyond leading order in $1/M$ the values for A, B, and C calculated in the static theory and NRQCD will not agree. The results for the static theory are basically obtained from those for NRQCD by expanding the internal quark propagators to a given order in $1/M$ before integrating. The results are then a truncated expansion in powers of $1/M$ of the expressions for A, B and C in NRQCD. If Ma is sufficiently large the expansion will be very convergent and the two theories will give very similar results. As Ma is reduced, the coefficients in the static theory will diverge earlier than those in NRQCD. This gives the latter theory a larger window in principle in which perturbation theory is accurate. How large this window is for either theory is yet to be determined.

We give results for A, B, and C for NRQCD on an infinite lattice in Tables I–III. We have chosen values of Ma appropriate to b and c quarks at $a = 1.0$ GeV^{-1} ($\beta \sim 5.7$) and for b quarks at $a = 0.5$ GeV^{-1} ($\beta \sim 6.0$). For values of $Ma < 3$ (c quarks at a=1.0 GeV^{-1} and b quarks at a=0.5 GeV^{-1}) we have used the action of Eq. (10). We have not treated c quarks at a=0.5 GeV^{-1} since this would require using n=3 in Eq. (9).

We also give results for finite spatial volumes $8 \times 8 \times 16$ and 16^3 to estimate finite-volume effects. We have not studied the case of a finite-size lattice in the time direction. Since the evolution equations can be continued for an arbitrary number of lattice time units, it is possible to take the effective time extent of the lattice for the

TABLE I. Results for the energy shift aA in lattice units. The error in the infinite-volume results is ± 0.0002 and the estimated error in the finite-volume results is ± 0.005. The values for Ma are chosen to cover the range of possible values for the b- and c-quark masses. 5 and 4.7 are appropriate for b quarks at a=1.0 GeV^{-1} and 2.5 and 2.35 at a=0.5 GeV^{-1}. 1.8 and 1.5 are values for the c quark at a=1.0 GeV^{-1}.

	Ma	aA_T	aA_S	aA
∞ volume	∞	−0.1684	0.0	−0.1684
	5	−0.1472	−0.0603	−0.2075
	4.7	−0.1461	−0.0641	−0.2102
	2.5	−0.1383	−0.1104	−0.2487
	2.35	−0.1374	−0.1167	−0.2541
	1.8	−0.1333	−0.1476	−0.2809
	1.5	−0.1314	−0.1727	−0.3041
$8 \times 8 \times 16$	5	−0.139	−0.059	−0.198
	4.7	−0.136	−0.0634	−0.199
	1.8	−0.126	−0.165	−0.291
	1.5	−0.123	−0.198	−0.321
16^3	2.5	−0.138	−0.120	−0.258
	2.35	−0.137	−0.128	−0.265

TABLE II. Results for the mass renormalization B. The error in the infinite-volume results is ± 0.0003 and the estimated error in the finite spatial volume results is ± 0.002. The significance of the different values of Ma is described in the caption to Table I.

	Ma	B
∞ volume	∞	0.2370
	5	0.2509
	4.7	0.2517
	2.5	0.3194
	2.35	0.3243
	1.8	0.3484
	1.5	0.3688
$8 \times 8 \times 16$	5	0.284
	4.7	0.283
	1.8	0.392
	1.5	0.413
16^3	2.5	0.347
	2.35	0.351

quark fields to be very long in numerical simulations if necessary. It is only the gluon fields which see a finite-size lattice in the time direction.

To obtain actual values for the $O(g^2)$ contributions we must multiply them by g^2 and there is some ambiguity in doing this. Recent work [9] has suggested that we should choose a renormalization scheme in which the heavy-quark potential at momentum transfer q has no $O(g^4)$ contribution in perturbation theory. It is hoped that this will mean $O(g^4)$ terms in other quantities will then be small also. The scheme has a physical motivation and gives good agreement between numerical calculations and $O(g^2)$ lattice perturbation theory for a number of different quantities. It will be the scheme we adopt here. The expansion parameter $g_V(q^2)$ is then given by the usual two-loop formula where Λ_V is $46.08\Lambda_{\text{lattice}}$ and the scale q^2 is chosen as the logarithmically averaged scale for the process. We choose q^2 to be π/a since the quantities we calculate here (A and B) are ultraviolet divergent and therefore mainly sensitive to scales close to the cutoff. We find $g_V^2(\pi/a) = 1.9$ at $\beta = 5.7$ and $g_V^2(\pi/a) = 1.7$ at $\beta = 6.0$.

One consequence of absorbing potentially large $O(g^4)$ contributions into g^2 is that g^2 becomes much larger than g^2_{lattice} and more scale dependent. We hope that by doing this the perturbative series will be more convergent. A test will be provided by comparing perturbative results for (some of) the coupling constants of the nonrelativistic theory with those from numerical tuning to fit experiment.

TABLE III. Results for the heavy-quark wave-function renormalization on the lattice, Z, with the infrared logarithmic dependence subtracted out. The error in the infinite-volume results is ± 0.0002 and the estimated error in the finite spatial volume results is ± 0.002. The significance of the different values for Ma is described in the caption to Table I.

	Ma	Z
∞ volume	∞	0.0383
	5	0.0070
	4.7	0.0052
	2.5	−0.0101
	2.35	−0.0121
	1.8	−0.0208
	1.5	−0.0264
$8 \times 8 \times 16$	5	0.016
	4.7	0.014
	1.8	−0.003
	1.5	−0.005
16^3	2.5	−0.001
	2.35	−0.002

A. Energy shift

Calculation of the energy shift A is straightforward. The numerical results for Aa for different values of the quark mass Ma are given in Table I. A is broken into a contribution from temporal gluons A_T [Figs. 3(a) and 3(b)] and that from spatial gluons A_S [Figs. 3(c) and 3(d)]. This will become useful later.

All four diagrams in Fig. 3 contribute to Aa. As explained earlier, the external quark momentum pa is set to zero and the integration over gluon momentum ka is done numerically. The gluon mass λ can be set to zero when evaluating the integrals since Aa is infrared finite. To obtain results on a finite spatial volume, we do the integration over $k_0 a$ analytically and sum over the spatial momenta $\mathbf{k}a$. We use periodic spatial boundary conditions, since they are generally used in numerical simulations. That means, however, that we must reintroduce the gluon mass to avoid a divergent contribution from $\mathbf{k}a = 0$. Provided $\lambda^2 a^2$ is larger than the smallest nonzero value for $\mathbf{k}^2 a^2$ on that volume we can safely extrapolate the results as a function of $\lambda^2 a^2$ to $\lambda^2 a^2 = 0$.

We have checked that the results agree with those of the leading-order static theory [2] in the $Ma \to \infty$ limit. It is in fact quite instructive to study the lattice integrals for A in this limit. Only Figs. 3(a) and 3(b) contribute. The sum of these diagrams is given by the integral

$$-\frac{2}{3}\int_{-\pi}^{\pi}\frac{d^4k}{(2\pi)^4}\frac{1}{4\sum_\mu[\sin(k_\mu/2)]^2}\left(\frac{2\exp(-ik_0)}{\exp(-ik_0)-1+\epsilon}-1\right), \tag{12}$$

where $\epsilon \sim 1/Ma$ and k replaces ka. Combining terms and symmetrizing the denominator with respect to k_0 shows that the resulting integral is odd in k_0 except for pieces proportional to $1/Ma$. In fact these terms give a finite result even as $1/Ma \to 0$. This is seen by replacing the gluon propagator by the difference between itself and the gluon propagator evaluated at $k_0 = 0$ [10]:

$$\frac{1}{\Delta_g(k)} \rightarrow \frac{1}{\Delta_g(k)} - \frac{1}{\Delta_g(k_0=0)} + \frac{1}{\Delta_g(k_0=0)}$$
$$= \frac{-4[\sin(k_0/2)]^2}{\Delta_g(k)\Delta_g(k_0=0)} + \frac{1}{\Delta_g(k_0=0)} . \quad (13)$$

The piece with $[\sin(k_0/2)]^2$ in the numerator vanishes as $1/Ma \rightarrow 0$. The other piece is finite as $1/Ma \rightarrow 0$ and gives the result simply as the three-dimensional (3D) integral over the gluon propagator with $k_0 = 0$.

At finite Ma one can also derive a useful result. In that case the second term of Eq. (13) gives the same answer, independent of Ma, provided that we keep $\epsilon < 1$, i.e., that we use the $n = 2$ action when $Ma \leq 3$. This means that A_T has only weak dependence on Ma provided by the first term of Eq. (13).

In the $Ma \rightarrow \infty$ limit, Aa is simply a number: -0.1684. A is then linearly divergent as $a \rightarrow 0$. At finite Ma extra quadratic divergences are introduced by terms in Aa of the form $1/Ma$. These arise from the spatial tadpole diagram [Fig. 3(c)], for example. When Ma is so small that the $n = 2$ action must be used Aa contains $(1/Ma)^2$, i.e., cubic divergences. Since A is such an ultraviolet quantity and not sensitive to the infrared cutoff of the lattice volume, we do not expect large finite-size effects when a finite spatial lattice is considered. Table I shows that such effects are indeed small, growing as Ma is reduced.

From Table I we see that g^2A will be around -0.5 GeV at $\beta = 5.7$ and close to -1.0 GeV for b quarks at $\beta = 6.0$. This is small compared to the b quark mass but large compared to the energy splittings between states.

It is interesting to consider what the static theory would give for A. The results at $O(1/M)$ are readily obtained as part of our calculation. The static theory would have the same temporal quark-gluon vertices as in NRQCD (see Fig. 1) but a quark propagator with the kinetic energy term replaced by ϵ. There would be an additional vertex of the form $p^2/2m$ that could appear once [to $O(1/M)$] on the internal quark line of Fig. 3(a).

Figure 3(a) provides a useful illustration of the differences between the two theories. If we replace the lattice sine functions by their continuum counterparts, we can do the integrals analytically. NRQCD would then give $-2M\ln(1 + \Lambda/2M)$ where the static theory would give $-\Lambda + \Lambda^2/4M$ to $O(1/M)$. As an expansion in powers of $1/M$ the static theory result is clearly unreliable once $\Lambda/2M > 1$. Attempts to systematically improve the static theory by including higher orders in $1/M$ will have problems if perturbative coefficients change drastically from one order to the next.

On the lattice Fig. 3(a) combines with the temporal tadpole which is the same for the two theories and independent of M [Fig. 3(b)]. For comparison to the results of NRQCD we find for the static theory aA_T has the value -0.1477 at $Ma = 5$, -0.1271 at $Ma = 2.5$ and -0.0995 at $Ma = 1.5$ $O(1/M)$. The coefficient of the $1/M$ dependence in these results is 0.1035. This contrasts with NRQCD in which A_Ta is not strongly mass dependent, changing only by 10% as Ma changes by a factor of 3 in Table I.

The situation for the spatial gluon diagrams [Figs. 3(c) and 3(d)] is rather different. A_Sa vanishes as $Ma \rightarrow \infty$ and is strongly mass dependent. In NRQCD it varies as $1/Ma$ at large Ma. As we reduce Ma and have to modify the action for NRQCD, additional powers of $1/Ma$ are introduced into both diagrams by the new Feynman rules of Fig. 2. The additional terms are more divergent, but they enter with opposite sign to the previous terms. The resulting divergence is slightly less than $1/Ma$ over the range of masses in Table I. In the static theory only Fig. 3(d) gives a result at $O(1/M)$. Figure 3(c) is $O(1/M^2)$ and should be neglected when considering $1/M$ corrections. The results at $O(1/M)$ are then larger in magnitude than the results of NRQCD, since they scale as $1/Ma$ for all Ma. We obtain -0.0620 at $Ma = 5$, -0.1240 at $Ma = 2.5$, and -0.2066 at $Ma = 1.5$ for the static theory. The total result for aA is actually very similar for NRQCD and the static theory over the range of masses in Table I.

We have also calculated the energy shift in NRQCD by allowing the lattice spacing in the time direction, a_t, to be less than that in the spatial direction, a. For $a_t = a/n$, the results for the energy shift are basically unchanged as n is increased for fixed a. At $Ma = 5$, we found aA to be -0.2211, -0.2265, -0.2282 for $n = 2, 4, 8$, respectively, and at $Ma = 1.8$, the values of aA were -0.3155, -0.3304, -0.3351 for $n = 2, 4, 8$. These numbers are not significantly different from the $n = 1$ case.

B. Mass renormalization

The contribution to the mass renormalization B was much harder to calculate numerically. It is necessary to set the quark on shell and take the second derivative with respect to $\mathbf{p}a$ analytically. Attempts at setting the quark on shell numerically yielded inconsistent results.

First, $\exp(ip_0a)$ must be eliminated by use of the appropriate on-shell condition for the $n = 1$ or 2 action. This modifies the quark propagators with momentum $p - k$ for the diagrams of Figs. 3(a) and 3(c) as well as modifying the vertices for the temporal gluons for Figs. 3(a) and 3(b). After differentiation, $\mathbf{p}a$ is set to zero and the 4D integration over loop momentum k must be done.

One term contains the cube of the quark propagator and was hard to handle numerically. We used integration by parts with respect to k_0a to reduce it to the square of the quark propagator, which was then easy to integrate numerically. Another approach is to do the whole k_0a integration analytically. This is not hard, since the only pole inside the k_0a integral comes from the gluon propagator. The resulting 3D integral is easy to handle numerically. Both methods of doing the integral agree.

Another method is to calculate $B + C$ by setting p_0a to zero before differentiating with respect to $\mathbf{p}a$. This is a useful check on the results for B and C.

At finite Ma, B is logarithmically divergent as $a \rightarrow 0$ for the $n = 1$ action and linearly divergent when $n = 2$. The numerical results for B for the infinite volume case and for different spatial lattice volumes are given in

Table II. The results at finite volume were obtained with the same summation techniques which were used for A. B is again not very volume dependent.

The values for Bg^2 are quite large and change considerably with Ma. They amount to a 50% correction to the mass for b quarks and 70% for c quarks using $g_V^2 = 1.9$. The infinite-mass value for B is 0.2370. This corresponds to the $O(g^2)$ correction to the coefficient of the kinetic term, which is needed in the static effective theory on the lattice when working strictly to $O(1/M)$. It has not been calculated previously.

We have also calculated the value of B in NRQCD for temporal lattice spacing, $a_t = a/n$, as we did for the energy shift. We find $B = 0.1928, 0.1644, 0.1487$ for $n = 2, 4, 8$ at $Ma = 5$. At $Ma = 1.8$, $B = 0.2214, 0.1972, 0.1836$ for $n = 2, 4, 8$. Clearly, the size of the temporal lattice spacing relative to the spatial lattice spacing has a fairly strong effect on the mass renormalization, particularly at low masses. Using a smaller temporal lattice spacing could decrease the $O(g^2)$ contribution to the mass renormalization to 40% for c quarks.

C. Wave-function renormalization

The constant C is found by first differentiating with respect to the energy, ip_0a, and then setting $p_0 = 0$. Differentiation breaks C into two distinct pieces, one of which is identical to aA_T, where A_T is the temporal contribution to the energy shift. This is particularly easy to see if Fig. 3(a) is drawn with momentum $p - k$ going through the gluon propagator and k through the quark propagator. The integral becomes

$$-\frac{4}{3}\int_{-\pi}^{\pi}\frac{d^4k}{(2\pi)^4}\left(\frac{\exp\left[i(p_0a+k_0)\right]}{\Delta_q(k)\Delta_g(pa-k)}\right) . \tag{14}$$

Differentiation with respect to ip_0a gives two pieces: one from differentiating the numerator and one from differentiating the quark propagator. Since the numerator is simply proportional to $\exp(ip_0a)$, the first piece reproduces the contribution of this diagram to aA when p_0 is set to zero. When combined with the differential of the tadpole diagram, Fig. 3(b), we obtain exactly aA_T. The second piece from Fig. 3(a), obtained by differentiating the quark propagator, is combined with a similar piece from the diagram with spatial gluons, Fig. 3(c), to give a contribution we call Z. Thus $C = Z + aA_T$. In this section we calculate Z since A_T has been given before.

Z has an infrared divergence as the gluon mass λ is taken to zero. The coefficient of this divergence can be calculated analytically, because it comes from the region of integration where $\mathbf{k} \sim 0$ in Fig. 3(a). In this region we can expand all the sine functions of spatial momentum into their continuum counterparts and perform the integration. At $O(g^2)$ the infrared divergence is found to take the form

$$\frac{1}{12\pi^2}(-2\ln\lambda^2a^2) . \tag{15}$$

The lattice calculation of Z must reproduce the infrared divergence in this form and we have checked that it does. The coefficient of the divergence is the same as that obtained for the wave-function renormalization in the full relativistic theory and this confirms that they are reproducing the same low-energy behavior.

We subtract Eq. (15) from the numbers obtained to give an answer for Z which is finite as $\lambda \to 0$. These results are given in Table III. The numbers are all very small.

Our results for Z agree in the $Ma \to \infty$ limit with those calculated by Eichten and Hill [10]. However, our result for C is $C = Z + aA_T$, while they obtained $C = Z - aA_T$. This will be explained in Sec. IV.

In the large mass limit Z takes the value 0.0383. It is clear from Table III that $\dot{Z}$ is strongly mass dependent, even changing sign at small Ma. In the value for C, Z will be overwhelmed by aA_T.

The static theory results for Z to $O(1/M)$ are 0.00467, −0.02890, −0.07362 for quark masses in lattice units of 5, 2.5, and 1.5. The coefficient of the $1/M$ dependence in these results is 0.168. This is again a rather stronger mass dependence than the results in NRQCD. The total result for $C = Z + aA_T$, however, is very similar for the static theory and NRQCD.

For the case with different spatial and temporal lattice spacings ($a_t = a/n$), $Z = -0.0020, -0.0189, -0.0397$ for $n = 2, 4, 8$ and $Ma = 5$. For $Ma = 1.8$, $Z = -0.0433, -0.0567, -0.0748$, for $n = 2, 4, 8$. There is a significant change in Z as n is increased, but Z will still be much smaller than aA_T.

IV. DISCUSSION

When the $O(g^2)$ corrections are included the inverse propagator in lattice units becomes

$$\Delta_q - \Sigma = (1 - Cg^2)\left[\exp(ip_0a) - 1 - Aag^2 + (1 - Bg^2)\frac{4}{2Ma}\sum_i\left(\sin\frac{p_ia}{2}\right)^2\right] \tag{16}$$

for lattice regularized NRQCD. We must compare this to the result for full QCD in continuum Minkowski space. In the renormalization scheme (modified minimal subtraction scheme) $\overline{\text{MS}}$ we would have an inverse propagator at $O(g^2)$ of the form

$$(1 - C_{\text{cont}}g^2)[\not{p} - M(1 - \delta_{\text{cont}}g^2)] , \tag{17}$$

where $C_{\text{cont}} = [-4 + \ln(M^2/\mu^2) + 2\ln(M^2/\lambda^2)]/12\pi^2$ and $\delta_{\text{cont}} = (4 + 3\ln\mu^2/M^2)/12\pi^2$. The nonrelativistic expansion of Eq. (17) will agree with the result from NRQCD at small pa if we adjust the coefficients of the operators in the Lagrangian of NRQCD or, equivalently, add counterterms.

The NRQCD Lagrangian becomes

$$S_Q = a^3\sum_{\mathbf{x}t}\psi^\dagger_{\mathbf{x}t}\left(\Delta_4 - (1 + Bg^2)\sum_{j=1}^{3}\frac{\Delta_j\Delta_{-j}}{2M_Ra}\right)\psi_{\mathbf{x}t} . \tag{18}$$

The overall wave-function renormalization factor $(1 + Cg^2)/(1 + C_{\rm cont}g^2)$ is conventionally not included in the action. We work with the bare fields of Eq. (18) and later renormalize our measured values for the matrix elements of currents involving ψ. The energy shift Aag^2 is also not included in the action. It can be added afterwards to the masses obtained from the action of Eq. (18).

The kinetic term, however, must be renormalized in the action. If we work with a kinetic term of effective mass $M_R a/(1 + Bg^2)$ we will match a continuum calculation with a mass in the action of $M_R(1 + \delta_{\rm cont}g^2)$ and a renormalized or pole mass in its perturbative quark propagator of M_R. Of course we do not know the value of M_R, although presumably it is around 5 GeV for a b quark. We must therefore fix the effective mass in the kinetic term of NRQCD on the lattice by numerical tuning. Once the effective mass is obtained we can extract M_R, although we have seen that $(1+Bg^2)$ is rather large for this to be reliable.

A value for M_R leads in principal to a prediction for absolute hadron masses by applying a shift to the masses extracted from simulation. The shift is $M_R + Ag^2$ per quark. The shift of Ag^2 is required to cancel the perturbatively generated energy. Notice that A is negative so that masses calculated in numerical simulations with the NRQCD action of Eq. (18) will be positive. M_R is added from outside NRQCD, because for that theory the usual mass term has been removed. To match the energy per quark of the relativistic theory, we must have an energy in the nonrelativistic theory of $M_R + p^2/2M_R + \cdots$ so the added mass must be M_R. Since $2Ag^2$ is less than 20% of the Υ mass, the main uncertainty in the energy shift will be the uncertainty in the value of M_R and the size of any nonperturbative effects. Nevertheless a reasonably accurate prediction for absolute masses, to within 30%, could be obtained. This is in itself a useful test of the theory. For mass splittings, on the other hand, no energy shift is required, and they should be obtained much more accurately.

Thus we have to fix the lattice spacing and effective mass numerically in lattice NRQCD. This is actually much simpler than in the relativistic theory. The lattice spacing can be fixed essentially independently of the mass by using the s-p splitting. The effective mass in lattice units can be tuned by comparing the wave function at the origin to that extracted from experimental leptonic decay rates. An additional perturbative vertex renormalization factor is required for this comparison [11].

Now we will return to the ambiguity in the value for C noted at the end of Sec. III. The resolution of this ambiguity lies in a comparison of the evolution equations for the Green's function used in our calculation and that of Ref. [10]. Our evolution equation is given in Eq. (3). In Ref. [10] an alternative, but equally valid choice of the time derivative operator is used:

$$\psi^\dagger_x \Delta_{-4}\psi_x = \psi^\dagger_x \psi_x - \psi^\dagger_x U^\dagger_{x-\hat{4},4}\psi_{x-\hat{4}} \ . \tag{19}$$

This would lead in NRQCD to an evolution equation:

$$G_{\mathbf{x}t} = (1 + H)^{-1}(U^\dagger_{\mathbf{x}t,4}G_{\mathbf{x}t-1} + \delta_{t,0}\delta_{\mathbf{x},0}) \ , \tag{20}$$

$$G_{\mathbf{x}t} = 0, t < 0 \ . \tag{21}$$

If we write out the evolution equations step by step we will see a clear difference. For the version using Δ_4 we have

$$G_0 = 0 \ , \tag{22}$$

$$G_1 = U^\dagger_{0,4} \ , \tag{23}$$

$$G_2 = U^\dagger_{1,4}(1 - H_1)U^\dagger_{0,4} \ . \tag{24}$$

For the version using Δ_{-4} we have

$$G_0 = (1 + H_0)^{-1} \ , \tag{25}$$

$$G_1 = (1 + H_1)^{-1}U^\dagger_{0,4}(1 + H_0)^{-1} \ , \tag{26}$$

$$G_2 = (1 + H_2)^{-1}U^\dagger_{1,4}(1 + H_1)^{-1}U^\dagger_{0,4}(1 + H_0)^{-1} \ . \tag{27}$$

Counting powers of $(1-H)$ would lead to a different fit to the numerical results for a correlation function calculated using the two evolution equations. For Δ_4 one would use $\exp[-m(t-1)]$ and for Δ_{-4}, $\exp[-m(t+1)]$. This is also clear, as it must be, from performing a Fourier transform of the free quark propagator in momentum space [see Eq. (8)]. The results we provide in this paper refer to the evolution equation for Δ_4. We prefer this form since the numerical simulation is easier. From Eq. (27), the Δ_{-4} case requires a 3D inversion of the operator $(1+H)$. Nevertheless, both evolution equations should lead to the same physical results, for masses etc. The raw numerical results for amplitudes may look different but there will also be different renormalization constants to be applied. For example, the constant C calculated in this paper will be different for the Δ_{-4} case.

One situation where the two evolution equations must yield identical numerical results before renormalization is in the $Ma \to \infty$ limit. Then $H \to 0$ and both equations yield the same string of $U^\dagger$ matrices for $t > 0$. This is also the Green's function for the static effective theory to zeroth order in $1/M$. However, in this limit, the Δ_4 action yields a wave-function renormalization $C = Z + aA_T$ and the Δ_{-4} action gives $C = Z - aA_T$. The Δ_{-4} result follows simply from the fact that the Feynman rules for Eq. (20) have vertices of the form $\exp(-ip_0)$ rather than $\exp(ip_0)$. Differentiation with respect to p_0 then introduces a minus sign into the pieces of C which correspond with aA_T. It is straightforward to show that Z and aA_T have the same value.

Since the naive interpretation of C is that it is the wave-function renormalization, this result is at first sight disturbing. Since the numerical value of the quark propagator calculated on the lattice is the same in the two cases, this must also be true in perturbation theory; and in fact it is. As noted above, the exponent of the Green's function has a different t dependence in the two cases and this difference is exactly matched, in perturbation theory, by the difference in the wave-function renormalization. It was pointed out in Ref. [10] that changing the $t+1$ to t in the exponent of the Green's function changes the wave-function renormalization by a finite amount aA_T. Here the difference is between $t-1$ and $t+1$ and the effect is

to change C by two units of A_T. Thus to $O(g^2)$ we have

$$\frac{1}{1-Zg^2-aA_Tg^2}(1+aA_Tg^2)^{t-1}$$

$$=\frac{1}{1-Zg^2+aA_Tg^2}(1+aA_Tg^2)^{t+1}\ . \quad (28)$$

Higher orders in g^2 must also make this equality true. This leads one to suspect that the Z and A_T pieces of C may factorize.

One is still left with an ambiguity in numerical simulations. There a fit to an exponent of $t-1$ will give a different answer for the amplitude of some correlation function to one with a fit of $t+1$, even after the appropriate wave-function renormalization for that fit is used. The difference between $t-1$ and $t+1$ is equivalent to shifting two units of the mass for that correlation function into the amplitude. The mass will consist of aA_T plus a physical binding energy. The contribution of the physical mass will vanish as $a \to 0$ but can give a significant contribution at finite a. There will also be differences in the renormalization constants at higher orders in g^2 than those that have been calculated. It may be true that, based on some estimation of the large contributions to the renormalization constant, one can prefer one fit over the other [9].

V. CONCLUSIONS

We have calculated the mass and wave-function renormalization and the energy shift for heavy quarks in NRQCD. These values will be useful in numerical simulations involving heavy quarks. The values for the mass renormalization and energy shift are large at $O(g^2)$. Nevertheless they can be used for a prediction of absolute hadron masses from a numerical simulation. The wave-function renormalization C can be combined with the $O(\alpha_s)$ corrections to vertex operators to produce values for $O(\alpha_s)$ corrections to decay constants measured in the lattice simulation. These values will be reported in another paper [11].

The calculations reported here for NRQCD differ from previous calculations given for the static theory [10] by the inclusion of the kinetic term in the action. There is a significant mass dependence in all of the renormalization parameters we have calculated; a 50% change over the mass range from b quarks to c quarks is typical. We discuss results from two different methods of controlling instability in the high-momentum modes. The method currently used in numerical simulation is that of modifying the action. Another possible method for the future is to take a lattice with reduced temporal lattice spacing. The results for the renormalization parameters are similar in the two cases, although the latter method gives a significantly smaller mass renormalization.

We compare our results to the static theory in which the kinetic term is included as a perturbation to $O(1/M)$. Renormalization parameters in that case inevitably have a mass dependence such as $1/Ma$, and this is significantly stronger than the mass dependence of NRQCD in most cases. It may lead to an earlier breakdown in perturbation theory for the static effective theory as Ma is reduced, although we see no sign of that for the values of Ma that we have considered here. We find the results of the static theory at $O(1/M)$ to be significantly different from those of NRQCD for individual pieces of the renormalization constants but in the total energy shift and wave-function renormalization these differences tend to cancel.

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