Relativistic corrections to gluon fragmentation into spin-triplet *S*-wave quarkonium

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We use the NRQCD factorization formalism to calculate the relativistic corrections to the fragmentation function for a gluon fragmenting into a spin-triplet *S*-wave heavy quarkonium. We make use of the gauge-invariant formulation of the fragmentation function of Collins and Soper. The color-octet contribution receives a large, negative relativistic correction, while the color-singlet contribution receives a large, positive relativistic correction. The considerable decrease in the color-octet contribution requires a corresponding increase in the phenomenological value of the leading color-octet matrix element in order to maintain a fit to the Fermilab Tevatron data.

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I. INTRODUCTION

In the nonrelativistic QCD (NRQCD) factorization approach, the rate of semi-inclusive quarkonium production at large transverse momentum (p_T) is given as a sum of products of short-distance coefficients and NRQCD matrix elements [1]. The short-distance coefficients are calculable as perturbative series in the strong-coupling constant α_s, while the production matrix elements, at least so far, must be determined by comparison with experimental data. The field theoretic ingredients that form the basis for the NRQCD factorization approach for quarkonium production are the collinear factorization of hard-scattering processes at large p_T [2–4] and the decomposition of the factored semi-inclusive production rate into NRQCD operator matrix elements and short-distance coefficients [1]. The NRQCD factorization formalism predicts that the NRQCD matrix elements are universal (process independent), and it also leads to a set of rules [1] for the scaling of matrix elements and interactions with v, where v is the heavy-quark or heavy-antiquark velocity in the quarkonium rest frame. ($v^2 \approx 0.3$ for the J/ψ, and $v^2 \approx 0.1$ for the Υ.) The confrontations of these expected properties of the NRQCD factorization formulas with experimental data are among the key tests of the NRQCD approach.

The production of quarkonium at large p_T in $p\bar{p}$ collisions provides a particularly important test of the NRQCD factorization approach. At a p_T of several times the quarkonium mass, the quarkonium production cross section is dominated by a process in which a gluon fragments into a quarkonium [5]. Other processes are suppressed by at least $1/p_T^2$ in the cross section. Furthermore, the process in which the gluon fragments into the quarkonium through a color-octet heavy quark-antiquark ($Q\bar{Q}$) channel dominates because it is enhanced by a factor v^4/α_s^2 relative to the color-singlet process [6]. It was pointed out by Cho and Wise [7] that a quarkonium that is produced through the color-octet process should have a substantial transverse polarization. The reason for this transverse polarization is that the fragmenting gluon is nearly on its mass shell, and, hence, is nearly completely transversely polarized. In the color-octet fragmentation process, that polarization is passed on to a produced $Q\bar{Q}$ pair, which then evolves into a quarkonium state. According to the velocity-scaling rules of NRQCD [1], the evolution of the $Q\bar{Q}$ pair into a quarkonium state is dominated by non-spin-flip interactions, which preserve the transverse polarization. Spin-flip interactions are suppressed by at least v^2.

The prediction of substantial quarkonium transverse polarization at large p_T relies not only on the validity of the NRQCD factorization formulas for quarkonium production, but also on the universality of the NRQCD matrix elements and the velocity-scaling rules. Therefore, experimental measurements of the polarization prediction test many of the essential features of the NRQCD factorization formalism. Such measurements are also important in that they can discriminate between the NRQCD factorization approach and the color-evaporation model, which predicts zero polarization for the produced quarkonium.

There have been several calculations, based on the NRQCD factorization approach, of the polarization of the produced quarkonium as a function of p_T. These include calculations of J/ψ polarization at leading order in α_s [7], at next-to-leading order in α_s [8], and at next-to-leading order in α_s, including the effects of feeddown from ψ' and χ_c states [9]; calculations of ψ' polarization at next-to-leading order in α_s [8–11]; and calculations of Υ polarization at next-to-leading order in α_s [12]. These calculations are generally in agreement with each other, although they are subject to large theoretical uncertainties, which arise mainly from uncertainties in the color-octet NRQCD matrix elements. The Collider Detector at Fermilab (CDF) data for J/ψ and ψ' polarization [13] do not support either the prediction of substantial transverse polarization at large p_T or the prediction of increasing transverse polarization with increasing p_T. However, it must be said that only the points at the highest p_T are more than 1.5 standard deviations away from the predictions in Ref. [9]. In the case of the Υ polarization, the CDF data [14] agree with the prediction [12]. However, the experimental error bars are too large to allow one to draw firm conclusions about the presence of substantial transverse polarization.

In light of the possible discrepancy between the predic-

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tions for J/ψ and ψ' polarization and the CDF data, it seems worthwhile to investigate the sizes of uncalculated contributions to the theoretical cross sections. Among such contributions are relativistic corrections, which begin in relative order v^2. It is known in the case of quarkonium decay rates that such corrections can be of the same size as the leading contribution [15]. Investigations of relativistic corrections to quarkonium decays of order v^4 [16] suggest that the order-v^2 contribution gives the bulk of the correction to the leading contribution.

In this paper, we calculate the relativistic corrections of relative order v^2 to the short-distance coefficients of both the color-octet and color-singlet terms in the fragmentation function for a gluon to fragment into a spin-triplet quarkonium state. We carry out the calculation at leading order in α_s. In computing the short-distance coefficients, we make use of the Collins-Soper definition of the fragmentation function in terms of a quantum chromodynamic (QCD) operator matrix element [17]. In carrying out this calculation, we confirm the results for the short-distance coefficients at leading order in v [5]. As a check of our methods, we also compute the correction of relative order v^2 to the three-gluon decay rate of a spin-triplet quarkonium state and find that it agrees with the results of Refs. [16,18]. We find that the relativistic correction to the color-octet fragmentation function is large and negative, while the correction to the color-singlet fragmentation function is large and positive.

The remainder of this paper is organized as follows. In Sec. II we review the Collins-Soper definition of the fragmentation function, and in Sec. III we use the NRQCD factorization formalism to write the expression for the fragmentation function in terms of NRQCD operator matrix elements and perturbatively calculable short-distance coefficients. In Sec. IV we describe the calculation of the short-distance coefficients. In Secs. V and VI we compute, respectively, the short-distance coefficients for the color-octet and color-singlet parts of the fragmentation function for a gluon fragmenting into a ${}^3S_1$ quarkonium state, through relative order v^2. Finally, we discuss the implications of our results in Sec. VII.

II. COLLINS-SOPER DEFINITION OF THE FRAGMENTATION FUNCTION

In this section we make use of the Collins-Soper definition of the fragmentation function [17] to write, in terms of NRQCD operator matrix elements and short-distance coefficients, the fragmentation function for a gluon to fragment into a quarkonium state. The Collins-Soper definition was first used in a calculation of a quarkonium fragmentation function by Ma [19].

Here, and throughout this paper, we use the following light-cone coordinates for a four-vector V:

$$V=(V^+,V^-,\boldsymbol{V}_\perp)=(V^+,V^-,V^1,V^2), \tag{1a}$$

$$V^+=(V^0+V^3)/\sqrt{2}, \tag{1b}$$

$$V^-=(V^0-V^3)/\sqrt{2}. \tag{1c}$$

The scalar product of two four-vectors V and W is then

$$V\cdot W=V^+W^-+V^-W^+-\boldsymbol{V}_\perp\cdot\boldsymbol{W}_\perp . \tag{2}$$

The fragmentation function $D_{g\to H}(z,\mu)$ is the probability for a gluon that has been produced in a hard-scattering process to decay into a hadron H carrying a fraction z of the $+$ component of the gluon's momentum. This function can be defined, in a light-cone gauge, in terms of the matrix element of a bi-local operator involving two gluon field strengths [20]. In Ref. [17], Collins and Soper introduced a gauge-invariant definition of the gluon fragmentation function:

$$\begin{aligned}D_{g\to H}(z,\mu)=&\frac{-g_{\mu\nu}z^{d-3}}{2\pi k^+(N_c^2-1)(d-2)}\int_{-\infty}^{+\infty}dx^-e^{-ik^+x^-}\\&\times\langle 0|G_c^{+\mu}(0)\mathcal{E}^\dagger(0^-)_{cb}\mathcal{P}_{H(zk^+,\mathbf{0}_\perp)}\mathcal{E}(x^-)_{ba}\\&\times G_a^{+\nu}(0^+,x^-,\mathbf{0}_\perp)|0\rangle.\end{aligned} \tag{3}$$

Here, $G_{\mu\nu}$ is the gluon field-strength tensor, k is the momentum of the field-strength tensor, and $d=4-2\epsilon$ is the number of space-time dimensions. There is an implicit average over the color and polarization states of the initial gluon. The parameter μ is the factorization scale, which appears implicitly through the dimensional regularization of the operator matrix element. The operator $\mathcal{P}_{H(P^+,\boldsymbol{P}_\perp)}$ is a projection onto states that, in the asymptotic future, contain a hadron H with momentum $P=(P^+,P^-=(M^2+P_\perp^2)/(2P^+),\boldsymbol{P}_\perp)$, where M is the mass of the hadron:

$$\mathcal{P}_{H(P^+,\mathbf{0}_\perp)}=\sum_X |H(P^+,\mathbf{0}_\perp)+X\rangle\langle H(P^+,\mathbf{0}_\perp)+X|. \tag{4}$$

The eikonal operator $\mathcal{E}(x^-)$ is a path-ordered exponential of the gluon field that makes the expression (3) gauge invariant by connecting the different space-time positions of the gluon field strengths:

$$\mathcal{E}(x^-)_{ba}=\mathrm{P}\exp\left[+ig\int_{x^-}^{\infty}dz^-A^+(0^+,z^-,0_\perp)\right]_{ba}, \tag{5}$$

where g is the QCD coupling constant, and $A^\mu(x)$ is the gluon field. Both A_μ and $G_{\mu\nu}$ are SU(3)-matrix valued, with the matrices in the adjoint representation. The manifest gauge invariance of expression (3) allows us to make use of the Feynman gauge in order to simplify the calculation.

The definition (3) is invariant under boosts along the longitudinal direction [17]. The fragmentation function is defined in a frame in which the transverse momentum of the hadron H vanishes: $\boldsymbol{P}_\perp=\mathbf{0}_\perp$. However, the fragmentation function is also invariant under boosts that change the transverse momentum of the hadron, while leaving the $+$ components of all momenta unchanged [17]. [This can be seen from the fact that the definition (3) is manifestly covariant, except for dependences on the $+$ components of some quantities and on the dummy variable x^-.] An explicit construction of such a Lorentz transformation is given in Appendix

A. However, for the purposes of this calculation, we find it convenient to work in the frame in which $\boldsymbol{P}_\perp = \boldsymbol{0}_\perp$.

In general, the fragmentation function (3) involves the long-distance dynamics of the evolution of gluon into a quarkonium state and, hence, is a nonperturbative quantity. However, we may evaluate the short-distance part of evolution of the gluon into a $Q\bar{Q}$ state H as a power series in α_s. A convenient set of Feynman rules for the perturbative expansion of Eq. (3) is given in Ref. [17]. For the purposes of this calculation, we need only the standard QCD Feynman rules and the special rule for the creation of a gluon by the operator $G_a^{+\nu}$ in Eq. (3). The latter rule, in momentum space, is a factor

$$+ik^+\left(g^{\nu\alpha} - \frac{Q^\nu n^\alpha}{k^+}\right)\delta_{ab}, \tag{6}$$

where k is the momentum of the field-strength tensor, Q is the momentum of the gluon, α and a are the vector and color indices, respectively, of the created gluon, and b is the color index of the eikonal line. In the absence of interactions with the eikonal line, $k = Q$.

In the definition (3), the transverse momentum of the hadron H is fixed. Therefore, the phase space is the product of the phase-space factors of all of the other final-state particles and the light-cone–energy-conserving delta function that is implied by the integration over x^- in Eq. (3):

$$d\Phi_n = \frac{4\pi M}{S}\,\delta\left(k^+ - P^+ - \sum_{i=1}^{n} a_i^+\right)\prod_{i=1}^{n}\frac{da_i^+ d^{d-2}\boldsymbol{a}_\perp}{2a^+(2\pi)^{d-1}}, \tag{7}$$

where S is the statistical factor for identical particles in the final state, a_i is the momentum of the ith final-state particle, and the product is over all of the final-state particles except H. Since we use nonrelativistic normalization for the hadron H, a factor $2M$ has been included in the phase space in order to cancel the relativistic normalization of H in the definition (3). In the remainder of this paper, we use nonrelativistic normalization for the hadron H and heavy quark Q and antiquark $\bar{Q}$, and we use relativistic normalization for all of the other particles.

III. NRQCD FACTORIZATION

The fragmentation of a gluon into a heavy-quarkonium state H involves many momentum scales, ranging from the factorization scale of the fragmentation function μ, which we assume to be of the order of the heavy-quark mass m or greater, to momenta much smaller than m, for which nonperturbative effects are large. The NRQCD factorization formalism allows one to make a systematic separation of momentum scales of order m and larger from scales of order mv or smaller. Following this approach [1], we write the fragmentation function of a gluon fragmenting into a heavy quarkonium in the form

$$D_{g\to H}(z,\mu) = \sum_n \left[d_n(z,\mu)\langle\mathcal{O}_n^H\rangle + d_n'(z,\mu)\langle\mathcal{P}_n^H\rangle\right] + O(v^3), \tag{8}$$

where the $\mathcal{O}_n^H$ and $\mathcal{P}_n^H$ are NRQCD operators, and the $d_n(z,\mu)$ and $d_n'(z,\mu)$ are short-distance coefficients. The first term on the right-hand side of Eq. (8) contains the operator matrix elements of leading order in v, and the second term contains the operator matrix elements of relative order v^2. The index n represents the quantum numbers of the operator. The matrix elements $\langle\mathcal{O}_n^H\rangle$ and $\langle\mathcal{P}_n^H\rangle$ are defined in the rest frame of H and are given, in the case of a $^3S_1$ state H, by the vacuum expectation values of the following four-quark operators:

$$\mathcal{O}_1^H = \chi^\dagger\sigma^i\psi\sum_X |H+X\rangle\langle H+X|\psi^\dagger\sigma^i\chi, \tag{9a}$$

$$\mathcal{O}_8^H = \chi^\dagger\sigma^i T^a\psi\sum_X |H+X\rangle\langle H+X|\psi^\dagger\sigma^i T^a\chi, \tag{9b}$$

$$\mathcal{P}_1^H = \frac{1}{2m^2}\left[\chi^\dagger\sigma^i\left(\frac{i}{2}\overleftrightarrow{\boldsymbol{D}}\right)^2\psi\sum_X |H+X\rangle\langle H+X| \times\psi^\dagger\sigma^i\chi + \text{H.c.}\right], \tag{9c}$$

$$\mathcal{P}_8^H = \frac{1}{2m^2}\left[\chi^\dagger\sigma^i T^a\left(\frac{i}{2}\overleftrightarrow{\boldsymbol{D}}\right)^2\psi\sum_X |H+X\rangle\langle H+X| \times\psi^\dagger\sigma^i T^a\chi + \text{H.c.}\right], \tag{9d}$$

where m is the heavy-quark mass, ψ is the Pauli field that annihilates a Q, χ is a Pauli field that creates a $\bar{Q}$, and $\chi^\dagger\overleftrightarrow{\boldsymbol{D}}\psi = \chi^\dagger(\boldsymbol{D}\psi) - (\boldsymbol{D}\chi)^\dagger\psi$. The sum is over all final states that contain the specified quarkonium state H. The NRQCD matrix elements are nonperturbative in nature, but they are universal, in that the same matrix elements describe inclusive production of $^3S_1$ quarkonium states in other high-energy processes.

IV. SHORT-DISTANCE COEFFICIENTS

The short-distance coefficients in Eq. (8) are independent of the long-distance dynamics of hadronization and, consequently, they are independent of the hadronic state H. Therefore, they can be calculated by examining the fragmentation function for the case in which the state H is a free $Q\bar{Q}$ state. We take the momenta of the Q and $\bar{Q}$ to be $p = P/2 + q$ and $\bar{p} = P/2 - q$, respectively. The heavy quark has three-momentum $\boldsymbol{q}$ in the $Q\bar{Q}$ rest frame, and, so, the invariant mass of the $Q\bar{Q}$ state is $P^2 = 4E^2$, where $E = \sqrt{m^2 + \boldsymbol{q}^2}$. Since the momentum q is fixed, the phase space of the $Q\bar{Q}$ pair is that of a single particle with momentum P, and it is omitted in the phase-space integrations in the computation of the fragmentation function. The fragmentation function for this free $Q\bar{Q}$ state is

$$D_{g\to Q\bar{Q}}(z,\mu)=\sum_n [d_n(z,\mu)\langle\mathcal{O}_n^{Q\bar{Q}}\rangle+d_n'(z,\mu)\langle\mathcal{P}_n^{Q\bar{Q}}\rangle] + O(v^3). \tag{10}$$

The definitions of the NRQCD matrix elements $\langle\mathcal{O}_n^{Q\bar{Q}}\rangle$ and $\langle\mathcal{P}_n^{Q\bar{Q}}\rangle$ are same as those in Eq. (9), except for the replacement $H\to Q\bar{Q}$. The short-distance coefficients $d_n(z,\mu)$ and $d_n'(z,\mu)$, which are common to both Eq. (8) and Eq. (10), can be obtained by comparing a perturbative calculation of the fragmentation function on the left-hand side of Eq. (10) with a perturbative calculation of the NRQCD matrix elements on the right-hand side of Eq. (10). While the fragmentation function and the matrix elements in Eq. (9) may both display sensitivity to long-range (infrared) interactions, that sensitivity cancels in the short-distance coefficients.

In determining the coefficients of $\langle\mathcal{O}_n^{Q\bar{Q}}\rangle$ and $\langle\mathcal{P}_n^{Q\bar{Q}}\rangle$ in $D_{g\to Q\bar{Q}}(z,\mu)$, it is convenient to make use of projection operators for the spin and color states of the $Q\bar{Q}$ pair. The projection operators for the $Q\bar{Q}$ pair in the color-singlet and color-octet configurations are

$$\Lambda_1=\frac{1}{\sqrt{N_c}}\delta_{ji}, \tag{11a}$$

$$\Lambda_8^a=\sqrt{2}T_{ji}^a, \tag{11b}$$

where i and j are the quark color indices in the fundamental (triplet) representation, a is the octet color index, and $N_c=3$. Spin-projection operators, accurate to all orders in v, have been given in Ref. [16].[1] For the spin-triplet state, the projection operator is

$$\Lambda(P,q,\epsilon^*)=\Lambda^\alpha(P,q)\epsilon_\alpha^*=N(\bar{\not p}-m)\not\epsilon^*\frac{\not P+2E}{4E}(\not p+m), \tag{12}$$

where ϵ is the polarization of the heavy-quark pair, and $N=[2\sqrt{2}E(E+m)]^{-1}$. Note that we use nonrelativistic normalization for the heavy-quark spinors. If $\mathcal{C}$ is the full QCD amplitude for a process, then the spin-triplet part of that amplitude is $\mathcal{M}=\mathrm{Tr}(\mathcal{C}\Lambda)$.

The S-wave part of $\mathcal{M}$ is

$$\mathcal{M}_{S\text{-wave}}=\mathcal{M}_0+\frac{\boldsymbol{q}^2}{m^2}\mathcal{M}_2+O(\boldsymbol{q}^4), \tag{13}$$

where the first two terms on the right-hand side of Eq. (13) are the leading and first subleading terms in the v expansion. Here,

[1]Projection operators that are accurate to lowest order in the nonrelativistic expansion have been given previously [21].

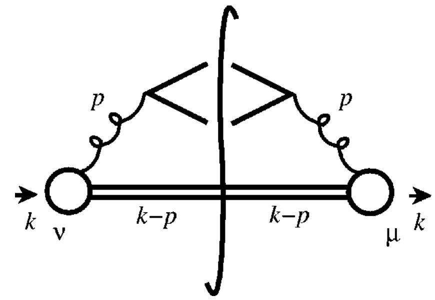

FIG. 1. Feynman diagram for the color-octet contribution at leading order in α_s to the fragmentation function for a gluon fragmenting into a color-octet spin-triplet $Q\bar{Q}$ pair.

$$\mathcal{M}_0=\mathcal{M}|_{\boldsymbol{q}\to\boldsymbol{0}}, \tag{14a}$$

$$\mathcal{M}_2=\frac{m^2 I^{\alpha\beta}}{2(d-1)}\frac{\partial^2\mathcal{M}}{\partial q^\alpha\partial q^\beta}\bigg|_{\boldsymbol{q}\to\boldsymbol{0}}, \tag{14b}$$

where

$$I^{\alpha\beta}=-g^{\alpha\beta}+P^\alpha P^\beta/(4E^2). \tag{15}$$

The matrix elements of the $Q\bar{Q}$ NRQCD operators are normalized as

$$\langle\mathcal{O}_1^{Q\bar{Q}}\rangle=2(d-1)N_c, \tag{16a}$$

$$\langle\mathcal{O}_8^{Q\bar{Q}}\rangle=(d-1)(N_c^2-1), \tag{16b}$$

$$\langle\mathcal{P}_n^{Q\bar{Q}}\rangle=\frac{\boldsymbol{q}^2}{m^2}\langle\mathcal{O}_n^{Q\bar{Q}}\rangle. \tag{16c}$$

The quantities that we calculate in this paper are all finite. Thus, we may put $d=4$ in Eqs. (3), (7), and (16).

V. COLOR-OCTET CONTRIBUTION

Let us calculate the color-octet contribution to the fragmentation of a gluon into a $Q\bar{Q}$ pair in full QCD. The Feynman diagram for the color-octet part of the fragmentation function in leading order in α_s is shown in Fig. 1. The circles represent the gluon field strengths and the double lines represent the eikonal operator. The momentum $k=(k^+,k^-,\boldsymbol{k}_\perp)$ flows into the circle on the left and out the circle on the right. The vertical line represents the final-state cut. In leading order in α_s, the final state consists of a $Q\bar{Q}$ pair with total momentum $P=(zk^+,P^2/(2zk^+),\boldsymbol{0}_\perp)$.

The Feynman diagram in Fig. 1 includes relativistic corrections to all orders in v. The phase-space element is obtained by setting $n=0$ and $S=1$ in Eq. (7):

$$d\Phi_0=\frac{4\pi M}{k^+}\delta(1-z). \tag{17}$$

The color-octet contribution can be extracted by tracing over the projection operator Λ_8^a [Eq. (11b)] on both the left-hand and right-hand sides of the cut. Summing over the color index a, we obtain the color factor $(N_c^2-1)/2$. The spin-triplet contribution can be extracted by tracing over the projection operator Λ^α [Eq. (12)] on the left-hand side of the cut and the projection operator Λ^β on the right-hand side of the cut. Multiplying by the prefactor in Eq. (3) and the phase-space element (17), we obtain

$$D_8^{Q\bar{Q}}(z)=-\frac{\pi\alpha_s M\mathcal{M}_{S\text{-wave}}^{\alpha\sigma}\mathcal{M}_{S\text{-wave}}^{\beta\tau*}}{8E^4}g^{\mu\nu}I_{\sigma\tau}\left(g_{\nu\alpha}-\frac{P_\nu n_\alpha}{k^+}\right)\times\left(g_{\mu\beta}-\frac{P_\mu n_\beta}{k^+}\right)\delta(1-z), \tag{18}$$

where $I_{\sigma\tau}$ is given in Eq. (15), and

$$\mathcal{M}_{S\text{-wave}}^{\alpha\sigma}=\mathrm{Tr}(\gamma^\alpha\Lambda^\sigma)_{S\text{-wave}}=-\sqrt{2}g^{\alpha\sigma}\left(1-\frac{\boldsymbol{q}^2}{6m^2}\right)+O(v^4). \tag{19}$$

In the last equality in Eq. (19), we have made use of Eq. (14). Contracting vector indices, factoring out the normalization of the octet matrix elements given in Eqs. (16b) and (16c), and setting $M=2E$, we obtain

$$\begin{aligned}D_8^{Q\bar{Q}}(z)&=\frac{\pi\alpha_s\delta(1-z)}{3(N_c^2-1)m^3}\left[\langle\mathcal{O}_8^{Q\bar{Q}}\rangle-\frac{11}{6}\langle\mathcal{P}_8^{Q\bar{Q}}\rangle\right]+O(v^4)\\&=d_8(z)\langle\mathcal{O}_8^{Q\bar{Q}}\rangle+d_8'(z)\langle\mathcal{P}_8^{Q\bar{Q}}\rangle+O(v^4),\end{aligned} \tag{20}$$

where $d_8(z)$ and $d_8'(z)$ are the short-distance coefficients. We obtain the contribution to the fragmentation function for a gluon fragmenting into a quarkonium H by replacing the $Q\bar{Q}$ operator matrix elements in Eq. (20) by H operator matrix elements:

$$D_8^H(z)=\frac{\pi\alpha_s\delta(1-z)}{3(N_c^2-1)m^3}\langle\mathcal{O}_8^H\rangle\left[1-\frac{11}{6}v_8^2+O(v^4)\right], \tag{21}$$

where

$$v_8^2=\langle\mathcal{P}_8^H\rangle/\langle\mathcal{O}_8^H\rangle. \tag{22}$$

Our result for the term of leading order in v in Eq. (21) is in agreement with the results of Refs. [22,23].

VI. COLOR-SINGLET CONTRIBUTION

Now let us calculate the color-singlet part of the fragmentation function for a gluon fragmenting into a $Q\bar{Q}$ pair in full QCD. The Feynman diagram for this process at leading order in α_s is shown in Fig. 2. We assign the momenta and polarization indices for the particles in this process as follows:

$$g^*(k,\alpha)\to Q\bar{Q}(P,\sigma)+g(a,\mu_a)+g(b,\mu_b), \tag{23}$$

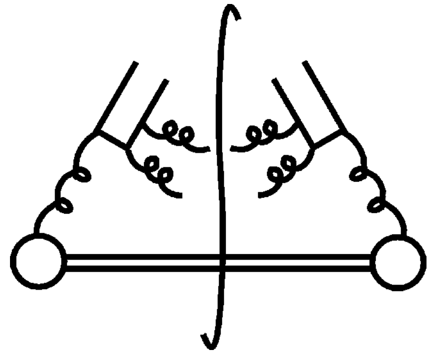

FIG. 2. One of the Feynman diagrams for the color-singlet contribution at leading order in α_s to the fragmentation function for a gluon fragmenting into a color-singlet spin-triplet $Q\bar{Q}$ pair. The other diagrams are obtained by permuting the connections of the gluons to the heavy-quark lines.

where k, P, a, and b are momenta and α, σ, μ_a, and μ_b are polarization indices. Owing to the color-singlet and spin-triplet quantum number of the $Q\bar{Q}$ pair, the final state must contain at least two gluons that couple to the heavy-quark line. Hence, in leading order in α_s, there are no diagrams for this process, in any gauge, in which a gluon couples to the eikonal line.

In the frame in which Eq. (3) is defined, we can choose the transverse direction so that

$$P=\left(zk^+,\frac{(2E)^2}{2zk^+},0,0\right), \tag{24a}$$

$$a=\left(yk^+,\frac{a_\perp^2}{2yk^+},a_\perp,0\right), \tag{24b}$$

$$b=\left(wk^+,\frac{b_\perp^2}{2wk^+},b_\perp\cos\phi,b_\perp\sin\phi\right), \tag{24c}$$

where ϕ is the azimuthal angle of b relative to a. The variables y and w are the light-cone fractions of final-state gluons: $y=a^+/k^+$, and $w=b^+/k^+$, with $z+y+w=1$. The phase-space element of the process can be obtained by making the substitutions $n=2$, $S=2$, $a_1=a$, and $a_2=b$ in Eq. (7). It is useful in carrying out the phase-space integration to express the variables $a_\perp$, $b_\perp$, and ϕ in terms of Lorentz-invariant dimensionless variables e_a, e_b, and x:

$$e_a=\frac{P\cdot a}{P^2}=\frac{1}{2}\left(\frac{za_\perp^2}{(2E)^2y}+\frac{y}{z}\right), \tag{25a}$$

$$e_b=\frac{P\cdot b}{P^2}=\frac{1}{2}\left(\frac{zb_\perp^2}{(2E)^2w}+\frac{w}{z}\right), \tag{25b}$$

$$x=\frac{a\cdot b}{P^2}=\frac{1}{2(2E)^2}\left(\frac{wa_\perp^2}{y}+\frac{yb_\perp^2}{w}-2a_\perp b_\perp\cos\phi\right). \tag{25c}$$

Note that only the invariant variable x depends on the angle ϕ. In terms of the variables e_a and e_b, the phase space is

$$d\Phi_2=\frac{M(2E)^4}{4z^2k^+(2\pi)^3}\int_\Phi, \tag{26a}$$

where

$$\int_\Phi \equiv \int_0^\infty de_a\int_0^\infty de_b\int_0^{1-z}dy \times\int_0^{2\pi}\frac{d\phi}{2\pi}\theta\left(e_a-\frac{y}{2z}\right)\theta\left(e_b-\frac{w}{2z}\right) \tag{26b}$$

and we have integrated over the azimuthal angle of a and the variable w. The θ functions in Eq. (26b) impose the requirement of the positivity of the variables $a_\perp^2$ and $b_\perp^2$. We defer the discussion of the change of variables from ϕ to x to Appendix B.

The color-singlet contribution can be extracted by tracing over the projection operator Λ_1 [Eq. (11a)] on both sides of the final state cut. Using charge-conjugation symmetry to relate diagrams involving permutations of the gluon connections to the heavy-quark lines (Fig. 2), we find that the color factor is

$$\left(\frac{d^{abc}}{4\sqrt{N_c}}\right)^2=\frac{(N_c^2-4)(N_c^2-1)}{16N_c^2}. \tag{27}$$

The spin-triplet contribution can be extracted by tracing over the projection operator Λ^α [Eq. (12)] on the left-hand side of the cut and the projection operator Λ^β on the right-hand side of the cut. Multiplying by the prefactor in Eq. (3) and the phase-space element (26a), we obtain

$$D_1^{Q\bar{Q}}(z)=\frac{(N_c^2-4)\alpha_s^3M}{32\pi z^{5-d}N_c^2}\int_\Phi\frac{\boldsymbol{\Xi}\cdot\mathcal{A}}{(1+2e_a+2e_b+2x)^2}, \tag{28}$$

where the scalar product in $\boldsymbol{\Xi}\cdot\mathcal{A}$ denotes the sum over all the repeated vector indices appearing in the product of the tensors $\boldsymbol{\Xi}$ and $\mathcal{A}$. These tensors are defined as

$$\boldsymbol{\Xi}=-g_{\mu\nu}g_{\mu_a\nu_a}g_{\mu_b\nu_b}I_{\sigma\tau}\left(g_{\nu\alpha}-\frac{k_\nu n_\alpha}{k^+}\right)\left(g_{\mu\beta}-\frac{k_\mu n_\beta}{k^+}\right), \tag{29a}$$

$$\mathcal{A}=\mathcal{M}\otimes\mathcal{M}^*\equiv\mathcal{M}_{S\text{-wave}}^{\alpha\mu_a\mu_b\sigma}\mathcal{M}_{S\text{-wave}}^{*\beta\nu_a\nu_b\tau}, \tag{29b}$$

$$\mathcal{M}^{\alpha\mu_a\mu_b\sigma}=\mathrm{Tr}\left[\gamma^\alpha\frac{1}{\not{p}-\not{k}-m}\gamma^{\mu_a}\frac{1}{-\bar{\not{p}}-\not{b}-m}\gamma^{\mu_b}\Lambda^\sigma(P,q)\right] +5\ \ \text{perm.}, \tag{29c}$$

where $I_{\sigma\tau}$ is given in Eq. (15), and the terms labeled "perm." in Eq. (29c) are generated by permuting the gluon momenta and polarization indices $(-k,\alpha),(a,\mu_a),(b,\mu_b)$. In Eq. (29), we have made use of the gauge invariance of the Collins-Soper form of the fragmentation function (3) to carry out the calculation in the Feynman gauge. We obtain the S-wave contributions of leading order in v and of relative order v^2 in Eq. (29b) by applying Eqs. (13) and (14) to the spin-triplet amputated amplitude (29c).

Substituting $N_c=3$, using Eq. (16) to factor out the NRQCD matrix element $\langle\mathcal{O}_1^{Q\bar{Q}}\rangle=6N_c$, and retaining terms through relative order v^2 in $\boldsymbol{\Xi}\cdot\mathcal{A}$ and in the phase-space factor $M=2E$, we obtain

$$\begin{aligned}D_1^{Q\bar{Q}}(z)&=\frac{5\alpha_s^3m}{2592\pi z}\int_\Phi\frac{F_0\langle\mathcal{O}_1^{Q\bar{Q}}\rangle+\left(\frac{1}{2}F_0+F_2\right)\langle\mathcal{P}_1^{Q\bar{Q}}\rangle}{(1+2e_a+2e_b+2x)^2}+O(v^4)\\&=d_1(z)\langle\mathcal{O}_1^{Q\bar{Q}}\rangle+d_1'(z)\langle\mathcal{P}_1^{Q\bar{Q}}\rangle+O(v^4),\end{aligned} \tag{30}$$

where $d_1(z)$ and $d_1'(z)$ are the short-distance coefficients, and

$$F_0=\boldsymbol{\Xi}\cdot(\mathcal{M}_0\otimes\mathcal{M}_0^*)|_{\boldsymbol{q}\to\boldsymbol{0}}, \tag{31a}$$

$$F_2=m^2\frac{\partial}{\partial\boldsymbol{q}^2}\left\{\boldsymbol{\Xi}\cdot\mathrm{Re}\left[\left(\mathcal{M}_0+2\frac{\boldsymbol{q}^2}{m^2}\mathcal{M}_2\right)\otimes\mathcal{M}_0^*\right]\right\}_{\boldsymbol{q}\to\boldsymbol{0}}. \tag{31b}$$

[Note that, although $\mathcal{M}_0$ and $\mathcal{M}_2$ are independent of $\boldsymbol{q}$, the factors $\boldsymbol{\Xi}$ in Eq. (31) introduce a dependence on $\boldsymbol{q}^2$.] We obtain the contribution to the fragmentation function for a gluon fragmenting into a quarkonium H by replacing the $Q\bar{Q}$ operator matrix elements in Eq. (30) by H operator matrix elements:

$$D_1^H(z)=\frac{5\alpha_s^3m\langle\mathcal{O}_1^H\rangle}{2592\pi z}\int_\Phi\frac{F_0+\left(\frac{1}{2}F_0+F_2\right)v_1^2}{(1+2e_a+2e_b+2x)^2}+O(v^4), \tag{32}$$

where v_1^2 is given by

$$v_1^2=\langle\mathcal{P}_1^H\rangle/\langle\mathcal{O}_1^H\rangle, \tag{33}$$

rather than by Eq. (22).

The evaluations of F_0 and F_2 in Eqs. (31) are straightforward, but quite involved. We compute F_0 and F_2 using REDUCE [24]. As a check, we carry out independent calculations using the FEYNCALC package [25] in MATHEMATICA [26]. By making the replacements $\boldsymbol{\Xi}\to-g_{\mu_a\nu_a}g_{\mu_b\nu_b}g_{\alpha\beta}I_{\sigma\tau}$ and $k^2\to0$ and multiplying by the appropriate factor, we also obtain the decay rate of the process $\Upsilon\to ggg$, including the relativistic correction. Our results agree with those in Refs. [16,18]. The rather lengthy expressions for F_0 and F_2 are given in a MATHEMATICA notebook file [27].

In order to evaluate the integrals in Eq. (32), we use Eq. (25c) to replace ϕ with x, as we have already mentioned, and we carry out the y integration analytically. This procedure is described in detail in Appendix B. The integration methods

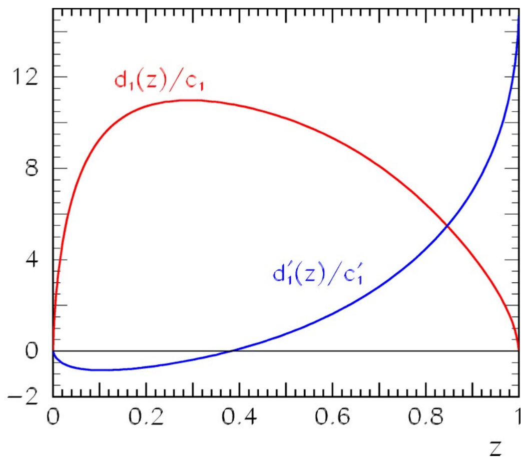

FIG. 3. The color-singlet short-distance coefficients $d_1(z)$ and $d_1'(z)$, which are defined in Eq. (30). The scaling factors in this figure are $c_1 = 10^{-4}\times\alpha_s^3/m^3$ and $c_1' = 10^{-3}\times\alpha_s^3/m^3$.

that we use are similar to those in Ref. [5]. However, in Ref. [5], the short-distance coefficient $d_1(z)$ is expressed as a two-dimensional integral, which is then evaluated numerically. In the present calculation, we carry out the integrations over the three variables e_a, e_b, and x numerically. This procedure allows one to extract information about the energy spectrum of the radiated gluons. The results of this numerical integration are presented in Fig. 3 and in Table I.

We note that the short-distance coefficient $d_1'(z)$ becomes negative for some values of z. The complete fragmentation function, to all orders in v, is an integral of the square of a quantity and is, therefore, positive. However, the individual contributions in the v expansion need not be positive.

We estimate the fragmentation probability by integrating the fragmentation function $D_1^H(z)$ over the longitudinal fraction z:

$$\int_0^1 dz D_1^H(z) = 8.29\times 10^{-4}\cdot\frac{\alpha_s^3}{m^3}\langle\mathcal{O}_1^H\rangle[1+2.45v_1^2+O(v^4)]. \tag{34}$$

Our result for the term of leading order in v in Eq. (34) is in agreement with the result of Ref. [5].

TABLE I. Numerical values of the color-singlet short-distance coefficients $d_1(z)$ and $d_1'(z)$, which are defined in Eq. (30). The scaling factors in this table are $c_1 = 10^{-4}\times\alpha_s^3/m^3$ and $c_1' = 10^{-3}\times\alpha_s^3/m^3$.

z	$d_1(z)/c_1$	$d_1'(z)/c_1'$
0	0	0
0.05	7.25	−0.746
0.10	9.27	−0.842
0.15	10.2	−0.808
0.20	10.7	−0.709
0.25	10.9	−0.564
0.30	11.0	−0.382
0.35	10.9	−0.162
0.40	10.7	0.0974
0.45	10.5	0.400
0.50	10.2	0.752
0.55	9.80	1.16
0.60	9.33	1.63
0.65	8.77	2.18
0.70	8.10	2.82
0.75	7.33	3.57
0.80	6.43	4.47
0.85	5.40	5.58
0.90	4.20	7.01
0.95	2.75	9.10
1	0	14.7

VII. DISCUSSION

We have computed the contributions of leading order in v and the relativistic corrections of relative order v^2 to the fragmentation function for a gluon to fragment into a ${}^3S_1$ heavy-quarkonium state. We have computed both the contribution in which the produced $Q\bar{Q}$ pair is in a color-octet state and the contribution in which the $Q\bar{Q}$ pair is in a color-singlet state. Our results of leading order in v agree with those of Refs. [22,23] for the color-octet contribution and with those of Ref. [5] for the color-singlet contribution. Our results for the corrections of relative order v^2 are new.

We estimate the relative sizes of the relativistic corrections for fragmentation into J/ψ by taking v_1^2 and v_8^2 from the Gremm-Kapustin relation [28]

$$v_1^2 = v_8^2 = \frac{M - 2m_{\rm pole}}{m_{\rm QCD}}, \tag{35}$$

where $m_{\rm pole}$ is the pole mass and $m_{\rm QCD}$ is the mass that appears in the NRQCD action. The Gremm-Kapustin relation follows from the equations of motion of NRQCD and is accurate up to corrections of relative order v^2. In the original work of Gremm and Kapustin [28], a relation was given only for v_1. In Eq. (35), we have included the Gremm-Kapustin relation for v_8, which can be derived in exactly the same manner as the Gremm-Kapustin relation for v_1. Dimensional regularization of the matrix elements $\langle\mathcal{P}_1^H\rangle$ and $\langle\mathcal{P}_8^H\rangle$ is implicit in the Gremm-Kapustin relation [29]. Taking $m_{\rm QCD} = m_{\rm pole} = 1.4$ GeV and $M_{J/\psi} = 3.097$ GeV, we obtain $v_1^2 = v_8^2 = 0.21$. One should regard this as only a rough estimate of the sizes of v_1 and v_8. In fact, for $m_{\rm pole}$ in the range 1.2 GeV $< m_{\rm pole} <$ 1.6 GeV, which corresponds to the latest Particle Data Group compilation [30], the values of v_1^2 and v_8^2 given by Eq. (35) can even become negative.[2] On the other hand, the estimate for v_1 that we obtain is in accor-

[2]Note that negative values of v_1^2 are allowed since, owing to the subtractions of power divergences that are implicit in dimensional regularization, the corresponding matrix element is not positive definite.

dance with expectations from the NRQCD velocity-scaling rules [1], and it lies in the central part of the range $0.03 < v_1^2 < 0.6$, which follows from a lattice calculation [31] under the assumption that m_c lies in the range 1.2 GeV$< m_c$ < 1.6 GeV. Inserting $v_1^2 = v_8^2 = 0.21$ into Eqs. (21) and (34), we find that the relativistic corrections change the short-distance coefficients for the color-octet contribution and the color-singlet contribution by about -40% and 50%, respectively.

We see that, in the case of the J/ψ, the estimated relativistic corrections are quite large in comparison with the contributions of leading order in v^2. This is not unexpected, given that such large relativistic corrections also appear in charmonium decays.[3] Nevertheless, these large relativistic corrections cast some doubt on the validity of the v expansion for charmonium. One can hope that, as is the case in charmonium decays [16], the corrections of relative order v^4 will turn out to be significantly smaller than the corrections of relative order v^2.

The value of the color-singlet matrix element $\langle \mathcal{O}_1^H \rangle$ is fixed by quarkonium decay rates. Therefore, the large relativistic correction to the short-distance coefficient of the color-singlet contribution to the fragmentation function will directly affect the theoretical predictions for quarkonium production rates. However, in the case of J/ψ production at the Tevatron, the color-singlet fragmentation contribution is less than 5% of the total theoretical prediction over a wide range of p_T [32–34]. Therefore, the relativistic correction to the color-singlet short-distance coefficient will have little effect on the predictions for either the J/ψ production rate or polarization at the Tevatron.

The color-octet matrix element $\langle \mathcal{O}_8^H \rangle$ in Eq. (21) is, at present, obtained by fitting the Tevatron data for J/ψ production to the complete theoretical expression, which is dominated at the largest values of p_T by the color-octet fragmentation contribution. Therefore, the large decrease in the short-distance coefficient for the color-octet contribution will result in a corresponding large increase in the fitted value of the matrix element $\langle \mathcal{O}_8^H \rangle$. The net result is that the phenomenology of J/ψ production at the Tevatron, for either the p_T distribution or the polarization, will be largely unaffected by the relativistic correction to the color-octet short-distance coefficient. Since, in leading order in α_s, the matrix element $\langle \mathcal{O}_8^H \rangle$ typically appears only in the fragmentation contribution to a process, we expect the phenomenology of other processes to be similarly unaffected. We note that, even with the increase in the fitted value of $\langle \mathcal{O}_8^H \rangle$ that would result from the relativistic correction, the value of that matrix element would still be somewhat smaller than is expected from the velocity scaling rules.[4] However, the relativistic correction may be important in comparing phenomenological values of $\langle \mathcal{O}_8^H \rangle$ with future lattice calculations.

[3]See, for example, Ref. [16].

[4]See, for example, Ref. [32] for fitted values of the matrix elements.

ACKNOWLEDGMENTS

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APPENDIX A: LORENTZ TRANSFORMATION FOR THE FRAGMENTATION FUNCTION

We wish to construct a Lorentz transformation that changes the transverse components of the hadron's momentum while leaving the $+$ components of all four-vectors unchanged. We will construct a particular transformation from a frame in which the fragmenting gluon has vanishing transverse momentum to a frame in which the quarkonium has vanishing transverse momentum. Such a transformation was already discussed in Ref. [17]. Here, we give an explicit construction.

Given a basis set of four linearly independent four-vectors that span the four-dimensional space-time, a transformation is a Lorentz transformation if and only if it leaves all scalar products of the basis four-vectors invariant. Using the notation $V=(V^+,V^-,V^1,V^2)$, we choose for our basis set in the original Lorentz frame

$$k=\left(k^+,\frac{k^2}{2k^+},0,0\right), \tag{A1a}$$

$$p=\left(zk^+,\frac{p^2+p_\perp^2}{2zk^+},p_\perp,0\right), \tag{A1b}$$

$$n=(0,1,0,0), \tag{A1c}$$

$$e_2=(0,0,0,1), \tag{A1d}$$

where we have taken the 1 direction to be along $\boldsymbol{p}_\perp$. We assume that n is invariant under the Lorentz transformation, which implies that the $+$ components of all four-vectors are also invariant. We also assume, for simplicity, that e_2 is invariant. Then, the transformed basis vectors are

$$k'=\left(k^+,\frac{k^2+p_\perp^2/z^2}{2k^+},\frac{-p_\perp}{z},0\right), \tag{A2a}$$

$$p'=\left(zk^+,\frac{p^2}{2zk^+},0,0\right), \tag{A2b}$$

$$n'=(0,1,0,0), \tag{A2c}$$

$$e_2'=(0,0,0,1). \tag{A2d}$$

The transformed vectors are completely fixed by the requirement that all of the scalar products be invariant under the transformation and the requirements that $\boldsymbol{p}'_\perp=\boldsymbol{0}_\perp$, $n'=n$, and $e'_2=e_2$.

Using Eqs. (A1) and (A2), we can construct an explicit transformation matrix L in the light-cone basis $\overline{n}=(1,0,0,0)$, $n=(0,1,0,0)$, $e_1=(0,0,1,0)$, and $e_2=(0,0,0,1)$. L is defined by $V'=LV$, where V is any four-vector, expressed as a column vector. It follows that L is given in terms of the untransformed and transformed light-cone basis vectors by

$$L=\begin{pmatrix} \overline{n'}\cdot n & n'\cdot n & e'_1\cdot n & e'_2\cdot n \\ \overline{n'}\cdot\overline{n} & n'\cdot\overline{n} & e'_1\cdot\overline{n} & e'_2\cdot\overline{n} \\ -\overline{n'}\cdot e_1 & -n'\cdot e_1 & -e'_1\cdot e_1 & -e'_2\cdot e_1 \\ -\overline{n'}\cdot e_2 & -n'\cdot e_2 & -e'_1\cdot e_2 & -e'_2\cdot e_2 \end{pmatrix}. \tag{A3}$$

From Eq. (A1), we see that the light-cone basis vectors can be written in terms of k, p, n, and e_2 as

$$\overline{n}=\frac{1}{k^+}\left(k-n\frac{k^2}{2k^+}\right), \tag{A4a}$$

$$n=n, \tag{A4b}$$

$$e_1=\frac{1}{2p_\perp}\left[2(p-zk)+n\frac{z^2k^2-p^2-p_\perp^2}{zk^+}\right], \tag{A4c}$$

$$e_2=e_2. \tag{A4d}$$

Then, the transformed light-cone basis vectors are

$$\overline{n'}=\frac{1}{k^+}\left(k'-n\frac{k^2}{2k^+}\right), \tag{A5a}$$

$$n=n, \tag{A5b}$$

$$e'_1=\frac{1}{2p_\perp}\left[2(p'-zk')+n\frac{z^2k^2-p^2-p_\perp^2}{zk^+}\right], \tag{A5c}$$

$$e'_2=e_2. \tag{A5d}$$

Substituting Eqs. (A4) and (A5) into Eq. (A3) and using Eqs. (A1) and (A2), we obtain

$$L=\begin{pmatrix} 1 & 0 & 0 & 0 \\ \frac{p_\perp^2}{2(p^+)^2} & 1 & -\frac{p_\perp}{p^+} & 0 \\ -\frac{p_\perp}{p^+} & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{A6}$$

The inverse transformation from the primed coordinates to the unprimed coordinates is given by $L^{-1}=L(p_\perp\to -p_\perp)$.

APPENDIX B: PHASE SPACE FOR THE COLOR-OCTET CONTRIBUTION

In this appendix we describe the manipulations that we carry out on the phase space for the color-singlet contribution to the fragmentation function [Eq. (26)] in order to put it into a form that is suitable for numerical integration. We write the phase-space integration as

$$\int_\Phi=\int_0^\infty de_a\int_0^\infty de_b\int_0^{1-z}dy\int_0^{2\pi}\frac{d\phi}{2\pi}\Theta, \tag{B1}$$

where $\Theta=\theta[e_a-(y/2z)]\theta[e_b-(w/2z)]$.

Since the integrand depends on ϕ only through the variable x [Eq. (25c)], it is an even function of ϕ. Therefore, we may restrict the range of ϕ to 0 to π and double the integrand: $\int_0^{2\pi}d\phi/(2\pi)\to\int_0^\pi d\phi/\pi$. In the range $0\leqslant\phi\leqslant\pi$, ϕ is a single-valued function of x. Consequently, we can make a change of integration variables in which we replace ϕ with x. Using Eq. (25), we rewrite x as

$$x=\frac{1}{2}(\alpha^2+\beta^2-2\alpha\beta\cos\phi), \tag{B2a}$$

where

$$\alpha=\sqrt{\frac{2w}{z}\left(e_a-\frac{y}{2z}\right)}, \tag{B2b}$$

$$\beta=\sqrt{\frac{2y}{z}\left(e_b-\frac{w}{2z}\right)}. \tag{B2c}$$

Note that, owing to the constraint Θ, α and β are real and positive. The Jacobian J for the change of the variables is given by

$$J=\left(\frac{dx}{d\phi}\right)^{-1}=\frac{1}{\alpha\beta\sin\phi}=\frac{z}{\sqrt{-A+2By-Cy^2}}=\frac{z}{\sqrt{C(y-y_-)(y_+-y)}}, \tag{B3a}$$

where

$$A=[zx-(1-z)e_a]^2, \tag{B3b}$$

$$B=-zx\left(e_a-e_b+\frac{1-z}{z}\right)+(1-z)e_a(e_a+e_b), \tag{B3c}$$

$$C=(e_a+e_b)^2-2x, \tag{B3d}$$

$$y_\pm=\frac{B\pm\sqrt{D}}{C}, \tag{B3e}$$

$$D = B^2 - AC$$
$$= 2z^2 x(2e_a e_b - x)\left[\frac{1-z}{z}\left(e_a + e_b - \frac{1-z}{2z}\right) - x\right]. \tag{B3f}$$

Using Eq. (B3a), we arrive at the following form for the phase space:

$$\int_\Phi = \int_0^\infty de_a \int_0^\infty de_b \int_0^{1-z} dy \int_0^\pi \frac{d\phi}{\pi}\Theta$$
$$= \int_0^\infty de_a \int_0^\infty de_b \int dx \int dy \frac{z\Theta}{\pi\sqrt{C(y-y_-)(y_+-y)}}, \tag{B4}$$

where we have interchanged the x and y integrations, and we have not yet specified the ranges of integration on the right-hand side of Eq. (B4).

Now let us work out the ranges of integration. The denominator on the right-hand side of Eq. (B4) has zeros at $y = y_+$ and $y = y_-$. (There is no zero at $C = 0$, since y_+ and y_- become infinite at that point.) As can be seen from Eq. (B3a), the denominator of Eq. (B4) is proportional to $\sin\phi$. Therefore, its zeros correspond to $\phi = 0$ and $\phi = \pi$, which are the end points of the ϕ integration. We conclude that the range of y is restricted to $y_- \leqslant y \leqslant y_+$. In order for y to have a nonzero range, we must have $D > 0$. This implies that x lies either below both zeros of $D(x)$ or above both zeros of $D(x)$. We now argue that the latter range is unphysical. Clearly, for x large enough, then Eq. (B2) has solutions only for y lying outside the physical region $0 \leqslant y \leqslant 1-z$ and $\Theta(y) = 1$. Furthermore, y is on the boundary of the physical region if and only if x is equal to a zero of $D(x)$. [To see this, note that the zeros of $D(x)$ occur precisely when the range of y vanishes. From Eq. (B2a), we see that the range of y vanishes if and only if $\alpha = 0$ or $\beta = 0$. But $\alpha = 0$ or $\beta = 0$ if and only if $y = 0$ or $y = 1-z$ or $\Theta = 0$, that is, if and only if y is on the boundary of the physical region.] Then, by continuity, we conclude that y lies in the physical region if and only if x is restricted to be less than either of the zeros of D. Therefore, we require that x satisfy

$$x \leqslant x^{\max}(z, e_a, e_b)$$
$$= \min\left[2e_a e_b, \frac{1-z}{z}\left(e_a + e_b - \frac{1-z}{2z}\right)\right]. \tag{B5}$$

Since, in this range of x, y automatically satisfies $0 \leqslant y \leqslant 1-z$ and $\Theta(y) = 1$, we can drop those explicit constraints on y. For fixed z, the constraint $\Theta = 1$ implies that $e_a + e_b \geqslant (1-z)/(2z)$. This constraint has already been satisfied by virtue of the constraint $x \leqslant x^{\max}$. However, for purposes of improving numerical-integration efficiency, we can explicitly impose it on the range of e_b. Taking all of the constraints on the integration variables into account, we have for the phase-space integration

$$\int_\Phi = \int_0^\infty de_a \int_{\max\{0,[(1-z)/2z]-e_a\}}^\infty de_b \int_0^{x^{\max}} dx$$
$$\times \int_{y_-}^{y_+} dy \frac{z}{\pi\sqrt{C(y-y_-)(y_+-y)}}. \tag{B6}$$

It turns out that there is no y dependence in the denominator of the integrand and that the numerator of the integrand is a polynomial in y of degree two. Therefore, the y integration is easily performed:

$$Y_n \equiv \int_{y_-}^{y_+} dy \frac{y^n}{\pi\sqrt{(y-y_-)(y_+-y)}}$$
$$= \sum_{r=0}^{r\leqslant n/2} \frac{n!\,\Gamma\left(r+\frac{1}{2}\right)B^{n-2r}(B^2-AC)^r}{r!(2r)!(n-2r)!\,\Gamma\left(\frac{1}{2}\right)C^n}. \tag{B7}$$

The explicit forms that are needed for the integrand in the present calculation are

$$Y_0 = 1, \tag{B8a}$$

$$Y_1 = \frac{B}{C}, \tag{B8b}$$

$$Y_2 = \frac{3B^2 - AC}{2C^2}. \tag{B8c}$$

In carrying out the integrations over z, e_a, e_b, and x numerically, we made use of the adaptive Monte Carlo routine VEGAS [35]. We also checked our results using the built-in numerical-integration package in MATHEMATICA [26]. Special care must be taken in carrying out the x integration numerically. In the limits $e_a \to 0$ or $e_b \to 0$, the range of the x integration vanishes. This can cause a large round-off error in the Monte Carlo integration. We avoided this problem by making a further change of variables $x = 2e_a e_b t$. The integration interval for t is $0 < t < x^{\max}/(2e_a e_b)$.

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