Next-to-Next-to-Leading-Order Charm-Quark Contribution to the *CP* Violation Parameter ϵ_K and ΔM_K

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The observables ϵ_K and ΔM_K play a prominent role in particle physics due to their sensitivity to new physics at short distances. To take advantage of this potential, a firm theoretical prediction of the standard-model background is essential. The charm-quark contribution is a major source of theoretical uncertainty. We address this issue by performing a next-to-next-to-leading-order QCD analysis of the charm-quark contribution η_{cc} to the effective $|\Delta S| = 2$ Hamiltonian in the standard model. We find a large positive shift of 36%, leading to $\eta_{cc} = 1.87(76)$. This result might cast doubt on the validity of the perturbative expansion; we discuss possible solutions. Finally, we give an updated value of the standard-model prediction for $|\epsilon_K| = 1.81(28) \times 10^{-3}$ and $\Delta M_K^{\rm SD} = 3.1(1.2) \times 10^{-15}$ GeV.

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Strangeness-changing neutral-current transitions play an important role in particle physics. The parameter ϵ_K, measuring indirect *CP* violation in the neutral kaon system, has received increased attention recently due to the discrepancy between the theoretical prediction and the experimental measurement [1–4]. In addition, together with the kaon mass difference ΔM_K, it provides strong constraints on many models of new physics.

Theoretical predictions for $\Delta M_K^{\rm SD}$ and ϵ_K are calculated in the framework of effective field theories, which allow us to separate short- and long-distance contributions, and to sum all terms which are enhanced by powers of large logarithms $\log(m_c^2/M_W^2)$ using the renormalization group. The relevant $|\Delta S| = 2$ effective Hamiltonian in the three-quark theory reads

$$\mathcal{H}^{\Delta S=2}_{f=3} = \frac{G_F^2}{4\pi^2} M_W^2 [\lambda_c^2 \eta_{cc} S(x_c) + \lambda_t^2 \eta_{tt} S(x_t) + 2\lambda_c \lambda_t \eta_{ct} S(x_c, x_t)] b(\mu) \tilde{Q}_{S2} + \text{H.c.}, \quad (1)$$

where G_F is the Fermi constant, $\lambda_i = V_{id}^* V_{is}$ comprises the Cabibbo-Kobayashi-Maskawa matrix elements, and $\tilde{Q}_{S2} = (\bar{s}_L \gamma_\mu d_L)^2$ is the leading local four-quark operator that induces the $|\Delta S| = 2$ transition, defined in terms of the left-handed s- and d-quark fields. The parameter $b(\mu)$ is factored out such that

$$\hat{B}_K = \frac{3}{2} b(\mu) \frac{\langle \bar{K}^0 | \tilde{Q}_{S2} | K^0 \rangle}{f_K^2 M_K^2}, \quad (2)$$

where f_K is the kaon decay constant, is a renormalization-group invariant quantity comprising the hadronic matrix element. It can be calculated on the lattice with high precision [5–9].

The loop functions S can be found, for instance, in [10]. The QCD and logarithmic corrections are contained in the η factors and are known at next-to-leading order (NLO) for the dominant top-quark contribution [$\eta_{tt} = 0.5765(65)$ [11]]. The relative suppression of the top-quark contribution by the small imaginary part of λ_t^2, relevant for ϵ_K, lets the charm-quark contributions compete in size. We have already performed a next-to-next-to-leading-order (NNLO) calculation of the charm-top contribution [$\eta_{ct} = 0.496(47)$ [12]]. Here, we focus on the charm-quark contribution, known until now at NLO, with a substantial error [$\eta_{cc} = 1.40(35)$ [3,13]]. It multiplies $S(x_c) = x_c + \mathcal{O}(x_c^2)$, where $x_c \equiv m_c^2/M_W^2$ and $m_c = m_c(m_c)$ is the $\overline{\rm MS}$ charm-quark mass. The Glashow-Iliopoulos-Maiani (GIM) mechanism cancels a potential large logarithm at leading order (LO).

The charm-quark contribution η_{cc} determines the short-distance part of the kaon mass difference $\Delta M_K^{\rm SD}$ and enters ϵ_K with a negative sign. The large remaining scale uncertainty at NLO hints at potentially sizable NNLO corrections; we confirm this expectation by an explicit calculation in this Letter.

Our calculation proceeds in three steps: determination of the initial conditions of the Wilson coefficients at the electroweak scale, renormalization-group evolution to the charm-quark scale, and matching onto the effective three-quark theory. The new result is the three-loop matching condition at the charm-quark scale.

The effective Hamiltonian in the five- and four-flavor theory relevant for η_{cc} reads

$$\mathcal{H}^{\Delta S=1}_{f=5,4} = \frac{4G_F}{\sqrt{2}} \sum_{i=+,-} C_i \sum_{q,q'=u,c} V_{q'd}^* V_{qs} Q_i^{qq'}. \quad (3)$$

Here the current-current operators are given by $Q_\pm^{qq'} = [(\bar{s}_L^\alpha \gamma_\mu q_L^\alpha) \otimes (\bar{q}_L'^\beta \gamma^\mu d_L^\beta) \pm (\bar{s}_L^\beta \gamma_\mu q_L^\beta) \otimes (\bar{q}_L'^\beta \gamma^\mu d_L^\alpha)]/2$, where α and β are color indices, and we define the evanescent operators in such a way that the anomalous dimension matrix is diagonal through NNLO [12,14]. The GIM mechanism cancels a contribution of the $|\Delta S| = 2$ Hamiltonian above the charm-quark scale; we verified explicitly that mixing of dimension-six into dimension-eight operators proportional to λ_c^2 does not occur above the charm-quark scale.

We take the initial conditions for $C_\pm$, obtained by a NNLO matching calculation at the electroweak scale, from Ref. [14]. The dimension-eight Wilson coefficient does not receive a contribution at the electroweak scale [15]. The running of $C_\pm$ to the charm-quark scale can be taken up to NNLO from [14].

At the scale $\mu_c = \mathcal{O}(m_c)$ the charm quark is removed from the theory as a dynamical degree of freedom. Requiring the equality of the Green's functions in both theories at μ_c leads to the matching condition

$$\sum_{i,j=+,-} C_i C_j \langle Q_i Q_j \rangle = \frac{1}{8\pi^2} \tilde{C}_{S2}^{cc} \langle \tilde{Q}_{S2} \rangle, \tag{4}$$

which we use to determine the Wilson coefficient $\tilde{C}_{S2}^{cc}$, defined implicitly in (10) below. Here, angle brackets denote operator matrix elements between s- and d-quark external states. Writing $\langle \tilde{Q}_{S2} \rangle = r_{S2} \langle \tilde{Q}_{S2} \rangle^{(0)}$ and $\langle Q_i Q_j \rangle = m_c^2/(8\pi^2) d_{ij} \langle \tilde{Q}_{S2} \rangle^{(0)}$, and expanding all quantities in powers of $\alpha_s/(4\pi)$, we find the following contributions to the matching (a sum over $i, j = +, -$ is implied):

$$\begin{aligned}
\tilde{C}_{S2}^{cc(0)} &= m_c^2(\mu_c) C_i^{(0)} C_j^{(0)} d_{ij}^{(0)}, \\
\tilde{C}_{S2}^{cc(1)} &= m_c^2(\mu_c)[C_i^{(0)} C_j^{(0)} (d_{ij}^{(1)} - d_{ij}^{(0)} \tilde{r}_{S2}^{(1)}) + (C_i^{(1)} C_j^{(0)} + C_i^{(0)} C_j^{(1)}) d_{ij}^{(0)}], \\
\tilde{C}_{S2}^{cc(2)} &= m_c^2(\mu_c)[C_i^{(0)} C_j^{(0)} (d_{ij}^{(2)} - (d_{ij}^{(1)} - d_{ij}^{(0)} \tilde{r}_{S2}^{(1)}) \tilde{r}_{S2}^{(1)} - d_{ij}^{(0)} \tilde{r}_{S2}^{(2)}) + (C_i^{(1)} C_j^{(0)} + C_i^{(0)} C_j^{(1)})(d_{ij}^{(1)} - d_{ij}^{(0)} \tilde{r}_{S2}^{(1)}) \\
&\quad + (C_i^{(2)} C_j^{(0)} + C_i^{(1)} C_j^{(1)} + C_i^{(0)} C_j^{(2)}) d_{ij}^{(0)} + \frac{2}{3} \log\frac{\mu_c^2}{m_c^2} ((C_i^{(1)} C_j^{(0)} + C_i^{(0)} C_j^{(1)}) d_{ij}^{(0)} + C_i^{(0)} C_j^{(0)} d_{ij}^{(1)})].
\end{aligned} \tag{5}$$

The strong coupling constant α_s is defined in the three-quark theory throughout this Letter, and superscripts in brackets denote the order of the expansion in α_s. Furthermore, we expand the charm-quark mass defined at the scale μ_c, viz. $m_c(\mu_c)$, about $m_c(m_c)$, as in Ref. [14].

In order to evaluate the Eqs. (5), we compute the finite parts of one-, two-, and three-loop Feynman diagrams of the type shown in Fig. 1; the evanescent operators in the $|\Delta S| = 2$ sector have been chosen as in [12]. Our NLO result confirms the calculation by Herrlich and Nierste [16] for the first time. The three-loop matching calculation yields [we use the notation $\hat{d}_{ij}^{(2)} \equiv d_{ij}^{(2)} - (d_{ij}^{(1)} - d_{ij}^{(0)} \tilde{r}_{S2}^{(1)}) \tilde{r}_{S2}^{(1)} - d_{ij}^{(0)} \tilde{r}_{S2}^{(2)}$; note also that $\hat{d}_{+-}^{(2)} = \hat{d}_{-+}^{(2)}$]:

$$\begin{aligned}
\hat{d}_{++}^{(2)} = {} & \frac{1\,665\,873\,233}{8\,164\,800} - \frac{1573}{162} B_4 - \frac{133}{72} D_3 + \frac{49}{36} \zeta_2 l_c \\
& + \frac{4313}{216} l_c^2 - \frac{15\,059}{1296} l_c + \frac{210\,213}{560} S_2 - \frac{1501}{54} \zeta_2^2 \\
& - \frac{7\,567\,241}{204\,120} \zeta_2 - \frac{1\,697\,893}{7776} \zeta_3 + \frac{11\,575}{216} \zeta_4,
\end{aligned} \tag{6}$$

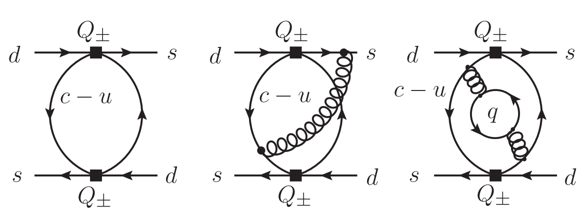

FIG. 1. Sample one-, two-, and three-loop diagrams contributing to the matching at the charm-quark scale. Loopy lines are gluons, and straight lines are quarks. The combination c-u arises from the GIM mechanism; q denotes any of the quarks u, d, s.

$$\begin{aligned}
\hat{d}_{+-}^{(2)} = {} & \frac{87\,537\,463}{1\,166\,400} + \frac{685}{162} B_4 - \frac{83}{72} D_3 + \frac{695}{36} \zeta_2 l_c \\
& - \frac{1475}{216} l_c^2 - \frac{57\,763}{1296} l_c - \frac{4797}{80} S_2 - \frac{791}{54} \zeta_2^2 \\
& + \frac{366\,569}{29\,160} \zeta_2 + \frac{57\,673}{7776} \zeta_3 - \frac{4999}{216} \zeta_4,
\end{aligned} \tag{7}$$

$$\begin{aligned}
\hat{d}_{--}^{(2)} = {} & \frac{2\,129\,775\,941}{8\,164\,800} + \frac{491}{162} B_4 + \frac{11}{72} D_3 + \frac{865}{36} \zeta_2 l_c \\
& + \frac{12\,533}{216} l_c^2 + \frac{171\,121}{1296} l_c + \frac{59\,121}{560} S_2 - \frac{517}{54} \zeta_2^2 \\
& + \frac{9\,261\,883}{204\,120} \zeta_2 - \frac{411\,709}{7776} \zeta_3 - \frac{7913}{216} \zeta_4,
\end{aligned} \tag{8}$$

where we defined $l_c = \log(\mu_c^2/m_c^2(\mu_c))$, ζ_n denotes Riemann's zeta function of n, and the remaining constants are defined in [17]. This result is new.

Since the calculation of the NNLO contributions to η_{cc} is quite complex, we checked our results in several ways. First of all the calculation of the $\mathcal{O}(10\,000)$ Feynman diagrams, the renormalization, and the matching calculation, has been performed independently by the two of us, using a completely different set of computer programs, leading to identical results. On the one hand we use QGRAF [18] for generating the diagrams; the evaluation of the integrals is then performed using the program packages Q2E, EXP, and MATAD [17,19,20]. On the other hand, all calculations have been performed using an independent setup, based on FEYNARTS [21], MATHEMATICA, and FIRE [22].

As a further check of our calculation, we verified that the matrix elements are finite and independent of the gauge-fixing parameter ξ. We have also checked analytically that η_{cc} is independent of the matching scales μ_W, μ_b, and μ_c

to the considered order of the strong coupling constant, by expanding the full solution of the renormalization-group equations about the respective matching scale.

The effective Hamiltonian valid below the charm-quark threshold contains only the single operator $\tilde{Q}_{S2}$. The renormalization-group evolution of the Wilson coefficient $\tilde{C}^{cc}_{S2}$ is described by the evolution matrix corresponding to the anomalous dimension of $\tilde{Q}_{S2}$:

$$\tilde{C}^{cc}_{S2}(\mu) = U(\mu, \mu_c)\tilde{C}^{cc}_{S2}(\mu_c). \qquad (9)$$

We express the coefficient η_{cc} in a scale- and scheme-independent way as

$$\eta_{cc} = \frac{1}{m_c^2(m_c)}\tilde{C}^{cc}_{S2}(\mu_c)[\alpha_s(\mu_c)]^{a_+}K_+^{-1}(\mu_c). \qquad (10)$$

The remaining scale dependence present in (9) is absorbed into

$$b(\mu) = [\alpha_s(\mu)]^{-a_+}K_+(\mu), \qquad (11)$$

where, up to second order in α_s,

$$K_+(\mu) = 1 + J_+^{(1)}\frac{\alpha_s(\mu)}{4\pi} + J_+^{(2)}\left(\frac{\alpha_s(\mu)}{4\pi}\right)^2, \qquad (12)$$

and the exponent $a_+ = 2/9$ is the so-called magic number for the operator Q_+ (the magic numbers as well as the matrices J, comprising the higher-order QCD contributions to the renormalization-group evolution, are defined, for instance, in [23]). This scale dependence is canceled by the corresponding scale dependence of the hadronic matrix element, order by order in perturbation theory. Consequently, our result is independent of μ_c up to and including terms of $\mathcal{O}(\alpha_s^2)$.

As a first estimate of the theoretical uncertainty of η_{cc} we study the residual scale dependence, using three different methods to evaluate the running strong coupling constant [14]. Matching at $m_c(m_c)$ and varying μ_c between 1 and 2 GeV (see Fig. 2) and μ_W between 40 and 160 GeV we find the following numerical value at NNLO,

$$\eta_{cc} = 1.86 \pm 0.53_{\mu_c} \pm 0.07_{\mu_W} \pm 0.06_{\alpha_s} \pm 0.01_{m_c}, \qquad (13)$$

where we also display the parametric uncertainties stemming from the experimental error on $\alpha_s(M_Z) = 0.1184(7)$ [24] and $m_c(m_c) = 1.279(13)$ GeV [25]. The dependence on the scale μ_b and on m_t is completely negligible [26].

Varying μ_c and μ_W in the same range as above, we find at NLO

$$\eta_{cc}^{\mathrm{NLO}} = 1.38 \pm 0.52_{\mu_c} \pm 0.07_{\mu_W} \pm 0.02_{\alpha_s}, \qquad (14)$$

where the error indicated by the subscript "μ_c" includes the effect of the three ways of determining α_s. We have included the parametric uncertainty related to α_s; the error resulting from m_c is negligible.

We find a substantial shift from NLO to NNLO for η_{cc}; furthermore, we observe that the NNLO calculation does

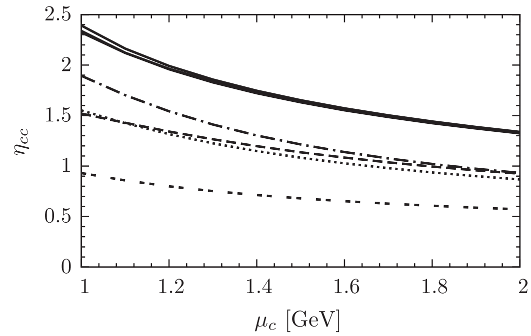

FIG. 2. η_{cc} as a function of μ_c, matching at $\mu = m_c(m_c)$ and fixing $\mu_W = 80$ GeV and $\mu_b = 5$ GeV. The LO result is represented by the double-dotted line. We also show the NLO value of η_{cc}, with the running α_s evaluated either by solving the renormalization-group equations numerically (dashed line), or by first computing the scale parameter Λ_{QCD}, either explicitly (dotted line) or iteratively (dash-dotted line)—see Ref. [36] for the details. The resulting uncertainty is sizable at NLO. The solid lines show the corresponding NNLO results; now the ambiguity is almost canceled, whereas the residual scale dependence is still large.

not reduce the residual scale dependence (see Fig. 2). This reveals a bad convergence behavior of the expansion of η_{cc} in α_s, even after having summed all terms proportional to $\alpha_s^n \log(m_c^2/M_W^2)^n$ and $\alpha_s^{n+1}\log(m_c^2/M_W^2)^n$ using the renormalization group. Some of the higher-order terms leading to the residual scale dependence are scheme dependent. In order to show that the large scale dependence is not artificial and to gain a better understanding of its origin, we expand the full solution of the renormalization-group equation. We find, up to terms cubic in α_s,

$$\begin{aligned}\eta_{cc}/(\alpha_s(m_c))^{2/9} = 1 &+ \alpha_s(m_c)(0.25 + 0.32L_c) \\ &+ (\alpha_s(m_c))^2(1.20 + 0.03L_b \\ &+ 0.22L_c + 0.27L_c^2),\end{aligned}$$

where $L_c = \log(m_c^2/M_W^2) = -8.28$, $L_b = \log(m_b^2/M_W^2) = -5.92$, and $\alpha_s(m_c) = 0.35$ at three-loop accuracy. Here we neglect the small terms proportional to L_b^2. This result is independent of the renormalization scale and the definition of the evanescent operators and depends implicitly only on the choice of the renormalization schemes used to determine $\hat{B}_K$ [cf. Eq. (10)], α_s, and the charm-quark mass. The large logarithmic terms proportional to powers of L_b and L_c are summed to all orders by the renormalization group in our full result, but the constant term of the NNLO correction is more problematic: it is almost twice as large as its NLO counterpart. Such large constant parts are expected to lead to a large residual sale dependence, as we indeed observe in Fig. 2.

The convergence of the series can be somewhat improved by expanding the square of the charm-quark mass multiplying η_{cc} in Eq. (1) in powers of α_s, noting that the charm-quark mass receives *negative* corrections, although the effect is not substantial at NNLO.

As a consequence of the discussion above, we propose the following temporary prescription: we take η_{cc} at $\mu_c = m_c$ as the central value, and as the theory uncertainty the absolute size of the NNLO correction and the residual scale dependence, added in quadrature. This leads to

$$\eta_{cc} = 1.87 \pm 0.76. \quad (15)$$

Compared to the NLO value $\eta_{cc}^{\rm NLO}$ (14), this corresponds to a positive shift of approximately 36%. The parametric uncertainty is essentially negligible with respect to the theoretical uncertainty.

Finally, we study the impact of η_{cc} at NNLO on the prediction of $|\epsilon_K|$ and $\Delta M_K^{\rm SD}$. We use the input values from [24], in particular $|V_{cb}| = 4.06(13) \times 10^{-2}$, plus $m_t(m_t) = 163.7(1.1)$ GeV [27], $m_b(m_b) = 4.163(16)$ GeV [25], $\lambda = 0.2255(7)$ [28], $\kappa_\epsilon = 0.923(6)$ [29], $\xi_s = 1.243(28)$ [30], $\eta_{tt} = 0.5765(65)$ [12], $\hat{B}_K = 0.737(20)$ [30,31], $\eta_{ct} = 0.496(47)$ [12], in the following formula (we express $\bar{\eta}$ and $\bar{\rho}$ through $\sin 2\beta$; for a discussion and definitions, see [1,10]):

$$|\epsilon_K| = \kappa_\epsilon C_\epsilon \hat{B}_K |V_{cb}|^2 \lambda^2 \bar{\eta}[|V_{cb}|^2(1-\bar{\rho})\eta_{tt}S(x_t) + \eta_{ct}S(x_c, x_t) - \eta_{cc}S(x_c)]. \quad (16)$$

Using the numerical values given above, we obtain

$$|\epsilon_K| = (1.81 \pm 0.14_{\eta_{cc}} \pm 0.02_{\eta_{tt}} \pm 0.07_{\eta_{ct}} \pm 0.05_{\rm LD} \pm 0.23_{\rm parametric}) \times 10^{-3}. \quad (17)$$

The first three errors correspond to η_{cc}, η_{tt}, η_{ct}, respectively. The error indicated by LD originates from the long-distance contribution, namely $\hat{B}_K$ and κ_ϵ, which account for 81% and 19% of the long-distance error, respectively. Half of the parametric error stems from $|V_{cb}|$ (49%), while all other contributions are well below 20%. All errors have been added in quadrature.

Compared to the prediction using the NLO value $\eta_{cc}^{\rm NLO}$, $|\epsilon_K^{\rm NLO}| = 1.90(27) \times 10^{-3}$, this corresponds to a shift of approximately -5%, and overcompensates the shift of $+3\%$ found in [12]. The large perturbative corrections are thereby partially mitigated in the observable ϵ_K.

Finally, we estimate the short-distance contribution to ΔM_K. Using [10]

$$\Delta M_K^{\rm SD} = \frac{G_F^2}{6\pi^2} f_K^2 B_K M_K M_W^2 \left(\lambda - \frac{\lambda^3}{2}\right)^2 \eta_{cc} x_c \quad (18)$$

we find $\Delta M_K^{\rm SD} = 3.1(1.2) \times 10^{-15}$ GeV, where the central value accounts for 89% of the measured value. We neglected the correction due to top quarks, of the order of 1%. The error is dominated by η_{cc} (86%) and B_K (6%). Unfortunately, the LD contributions to ΔM_K are poorly known; the discussion in Ref. [32] hints at a positive contribution. In addition, our calculation shows that also the SD contribution cannot be computed as reliably as thought previously, and thus the prediction of the total kaon mass difference suffers from large uncertainties.

We have performed the first NNLO QCD analysis of the charm-quark contribution η_{cc} to the $|\Delta S| = 2$ effective Hamiltonian $\mathcal{H}_{f=3}^{|\Delta S|=2}$. We confirm the analytical results for η_{cc} obtained at NLO in Ref. [16] for the first time.

The discrepancy between our standard-model prediction and the precisely measured experimental value $|\epsilon_K|^{\rm exp} = 2.228(11) \times 10^{-3}$ [24] could be interpreted as a tension within the standard model if we got a better control of the theoretical uncertainty. In view of the considerable residual scale dependence and the large NNLO shift, sizable corrections beyond NNLO may be expected.

Given the importance of the observable ϵ_K, an effort should be made to circumvent these difficulties. We see at least two possible ways to proceed: in the short run, one could make use of the cancellation of the scheme dependence between of the parameter B_K and the effective Hamiltonian. One could utilize this scheme dependence [which would affect the quantities J in Eq. (12)] to achieve a better convergence of η_{cc}. Recently, new lattice renormalization schemes have been employed in the determination of B_K [6,33]; they use nonexceptional momentum configurations, leading to better control over lattice uncertainties. Furthermore, they might lead to a better convergence at NNLO, as suggested by the good perturbative behavior of the continuum matching for the light-quark masses [34,35]. We encourage the investigation of the effects of these schemes also on the convergence of the series for η_{cc}, in particular, at NNLO. In the long run, the possibility of calculating the effects of a dynamical charm quark on the lattice might seem most promising and should be further studied.

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