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B^0-$\bar{B}^0$ Mixing in Unquenched Lattice QCD

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We present an unquenched lattice calculation for the B^0-$\bar{B}^0$ transition amplitude. The calculation, carried out at an inverse lattice spacing $1/a = 2.22(4)$ GeV, incorporates two flavors of dynamical quarks described by the $O(a)$-improved Wilson fermion action and heavy quarks described by nonrelativistic QCD. Particular attention is paid to the uncertainty that arises from the chiral extrapolation, especially the effect of pion loops, for light quarks, which we find could be sizable for the leptonic decay constant, whereas it is small for the B parameters. We obtain $f_{B_d} = 191(10)(^{+12}_{-22})$ MeV, $f_{B_s}/f_{B_d} = 1.13(3)(^{+13}_{-2})$, $B_{B_d}(m_b) = 0.836(27)(^{+56}_{-62})$, $B_{B_s}/B_{B_d} = 1.017(16)(^{+56}_{-17})$, and $\xi = 1.14(3)(^{+13}_{-2})$, where the first error is statistical, and the second is systematic, including uncertainties due to chiral extrapolation, finite lattice spacing, heavy quark expansion, and perturbative operator matching.

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The unitarity test for the Cabibbo-Kobayashi-Maskawa (CKM) matrix entered a new era with the *BABAR* and Belle measurements of the angle ϕ_1 [1,2]. The test requires the determination of the other angles and the sides of the unitarity triangle, the precision of the latter being limited by uncertainties in hadronic matrix elements. Lattice QCD in principle offers a model-independent calculation of such matrix elements. Those matrix elements provided by lattice calculations to date, however, are based on the quenched approximation, blindly hoping that quenching does not introduce large errors.

Simulations including creation and annihilation of a quark antiquark pair in the vacuum have become feasible only recently. In this Letter we present an unquenched lattice calculation of the hadronic matrix elements appearing in the B^0-$\bar{B}^0$ mixing amplitude, which is needed in the determination of the CKM matrix element $|V_{td}|$ from the mass difference ΔM_d [3]. The matrix element is parametrized as $\langle \bar{B}^0_q|\bar{b}\gamma_\mu(1-\gamma_5)q\bar{b}\gamma_\mu(1-\gamma_5)q|B^0_q\rangle \equiv \frac{8}{3}f^2_{B_q}B_{B_q}M^2_{B_q}$, where f_{B_q} is the B meson decay constant and B_{B_q} denotes the B parameter (q represents d or s quark). Our prime interest is to calculate B_{B_q}, as unquenched calculations of f_{B_q} are already available [4]. We include, however, the calculation of f_{B_q} to provide a consistent set of the matrix element for B^0-$\bar{B}^0$ mixing.

With current lattice calculations, systematic uncertainties due to the discretization error and the perturbative matching between continuum and lattice operators amount to 10%–20%. One may improve the accuracy of $|V_{td}|$ by studying the ratio $\Delta M_s/\Delta M_d$ if B_s-$\bar{B}_s$ mixing is measured. The relevant quantity is $\xi \equiv (f_{B_s}\sqrt{B_{B_s}})/(f_{B_d}\sqrt{B_{B_d}})$, where many of the systematic uncertainties cancel in the lattice calculation.

A remaining major uncertainty arises from the chiral extrapolation of the lattice simulation which is made with relatively heavy dynamical quarks. One may resort to chiral perturbation theory (ChPT) as a theoretical guide for the extrapolation. The problem is that the currently available lattice data do not show the logarithmic behavior expected from long-distance pion loops in ChPT [5]. It is in the scope of the present work to discuss the uncertainty in the matrix elements associated with the chiral extrapolation in the absence of the observable logarithmic behavior.

The calculation is carried out on the unquenched gauge configurations generated at $\beta = 5.2$ on a $20^3 \times 48$ lattice. Two flavors of dynamical quarks for the u and d quarks are simulated at five values of quark mass in the range $(0.7–2.9)m_s$ with m_s the physical strange quark mass. This corresponds to the pseudoscalar to vector mass ratio of 0.6–0.8. The hopping parameter chosen is $K_{\rm sea} =$ 0.1340, 0.1343, 0.1346, 0.1350, and 0.1355. For each sea quark mass, 1200 configurations are accumulated for measurements from 12 000 hybrid Monte Carlo trajectories separated by ten trajectories. The lattice spacing we adopt is determined from ρ meson mass and equals 2.22(4) GeV after the extrapolation to the chiral limit.

This value is consistent with $2.19(^{+7}_{-5})$ GeV from the Sommer scale r_0 assuming the physical value of 0.49 fm, and 2.25(5) GeV from f_K [with an additional $O(5\%)$ error from the perturbative matching]. This suggests that the large width of ρ may not seriously affect the chiral extrapolation of the ρ meson mass. Other details of the simulation are described in [6]. We adopt the lattice nonrelativistic (NRQCD) formalism [7,8] for heavy quarks. The nonperturbatively $O(a)$-improved Wilson action [9] is employed for both valence and sea light quarks.

We take five values of heavy quark mass m_Q ($am_Q =$ 1.3, 2.1, 3.0, 5.0, and 10.0) to cover $m_Q = 3$–20 GeV for the NRQCD action that contains all corrections of the order $1/m_Q$. We take the valence light quark mass set equal to the sea quark mass and then extrapolate to the physical u- and d-quark masses, unlike the "partially quenched analysis" often adopted in the literature. The strange quark is treated in the quenched approximation. There is an uncertainty in the determination of the strange quark mass depending upon which strange hadron is used as input. We take three values for the hopping parameter $K_s = 0.13465$, 0.13468, and 0.13491 and interpolate to $K_s(K) = 0.13486(3)$ (for the K meson as input) and $K_s(\phi) = 0.13471(4)$ (for the ϕ meson as input) [6]. The method to calculate f_B and the B parameter follows our previous studies in the quenched approximation [10,11].

Figure 1 shows the chiral extrapolation of the decay constants f_{B_q} expressed in terms of $\Phi_{f_{B_q}} \equiv f_{B_q}\sqrt{M_{B_q}}$ as a function of the pion mass squared. For f_{B_s}, the result is shown at $K_s = 0.134\,65$. In order to absorb the change of effective lattice scale that varies with $K_{\rm sea}$ at a fixed bare coupling β, both axes are normalized with r_0 determined from the heavy quark potential at each sea quark mass.

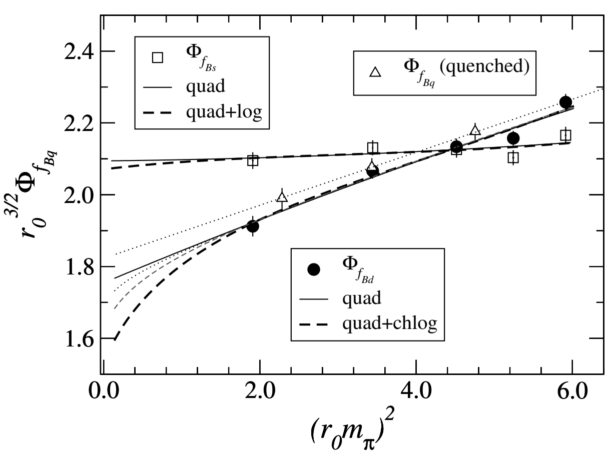

FIG. 1. Chiral extrapolation of $\Phi_{f_{B_d}}$ (filled circles) and $\Phi_{f_{B_s}}$ (open squares). The quadratic extrapolation is shown by solid lines, while the fits with the hard cutoff chiral logarithm are shown for $\mu = 300$ (dotted curves), 500 (thin dashed curve), and ∞ (thick dashed curve) MeV. Quenched results are also shown (triangles).

The heavy quark mass is interpolated to the b quark using the lattice data.

Open triangles show quenched results obtained at a similar lattice spacing $1/a = 1.83(2)$ GeV ($\beta = 6.0$) with the nonperturbatively improved Wilson quark action. Our observation that they lie close to the unquenched data (filled circles) implies that the B meson decay constant takes a similar value in quenched and two-flavor QCD if the scale is normalized by r_0. With the more conventional normalization of using the ρ mass, however, the unquenched values are higher by about 20% (see, e.g., [4]), as is seen by the fact that $r_0 m_\rho = 1.91(2)$ for $N_f = 2$ while it is 2.20(3) on the quenched lattice [6]. This is understood as systematic errors of the quenched approximation, with which the determination of the lattice scale depends on which physical quantity is the input. With the dynamical quarks these errors are significantly reduced, leading to a convergent determination of the lattice scale.

The solid line represents a linear plus quadratic fit in $(r_0 m_\pi)^2$, which describes the lattice data well. This fit, however, does not contain the chiral logarithmic term which is predicted by ChPT [12]:

$$\frac{\Phi_{f_{B_d}}}{\Phi^{(0)}_{f_{B_d}}} = 1 - \frac{3(1+3g^2)}{4}\frac{m_\pi^2}{(4\pi f)^2}\ln\frac{m_\pi^2}{\mu^2} + \cdots, \qquad (1)$$

where terms regular in m_π^2 are omitted, and the coupling g is the $B^* B\pi$ interaction in ChPT. Lattice calculations [13,14] give a value consistent with the empirical one measured for $D^* \to D\pi$ decay, $g = 0.59 \pm 0.01 \pm 0.07$ [15]. Although there is an uncertainty in translating the value at the $D^{(*)}$ meson to that at the infinitely heavy quark mass (where the heavy-light ChPT is formulated), we take $g = 0.6$ to estimate the effect of the chiral logarithm.

Let us here consider a simpler case. For the pion decay constant the one-loop logarithmic term is controlled by the number of dynamically active quark flavors N_f as $-(N_f/2)[m_\pi^2/(4\pi f)^2]\ln(m_\pi^2/\mu^2)$; no uncertain parameters such as g are involved. Thus, the test for the presence of the chiral logarithm is less ambiguous [5]. Our high statistics unquenched data, shown in Fig. 2, exhibit quite a linear behavior for $(r_0 m_\pi)^2 > 2$, i.e., $m_\pi > 500$ MeV; no appreciable curvature characteristic of the chiral logarithm is observed.

One may suspect that pions in the simulation are too heavy to validate the use of ChPT. Another possibility may be the effect of explicit chiral symmetry breaking of the Wilson quark action at finite lattice spacings, as was discussed recently in the context of ChPT by [16] (see also [17,18]). Here we explore the more naturally looking, former possibility that the pion loop is suppressed for heavy pions and that the chiral logarithm manifests itself only for sufficiently small sea quark masses. The authors of [19] proposed a model that incorporates such a behavior by introducing a hard cutoff regularization of the

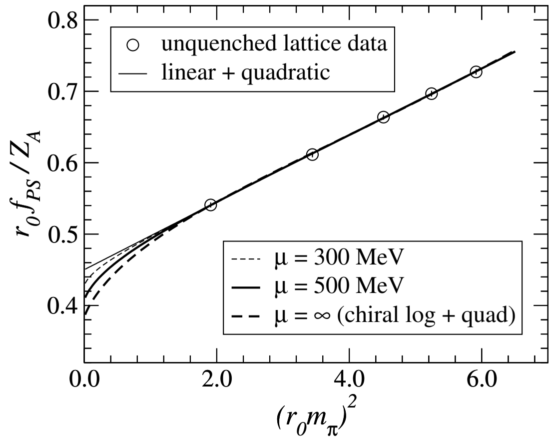

FIG. 2. Chiral extrapolation of f_π divided by the renormalization factor Z_A. The fits with the hard cutoff chiral logarithm are shown for $\mu = 300$ (thin dashed curve), 500 (thick curve), and ∞ (dashed curve) MeV.

one-loop ChPT calculation. This amounts to the replacement, $m_\pi^2 \ln m_\pi^2/\mu^2 \to m_\pi^2 \ln m_\pi^2/(m_\pi^2 + \mu^2)$, where μ is the scale of the hard cutoff, beyond which pion loop effects are suppressed. This function has to be understood as a model when used above the cutoff μ. We may use this model to explore the possible range of uncertainties consistent with the lack of curvature in our data.

Curves in Fig. 2 illustrate the chiral extrapolation using the cutoff logarithm plus a quadratic term. All curves are consistent with the lattice data, and they deviate from the polynomial only in the small mass region. The $\mu = \infty$ limit corresponds to the usual chiral logarithm function plus a quadratic term, for which the curvature cancels between the logarithmic and quadratic terms in the region of simulations while giving a large effect below $(r_0 m_\pi)^2 < 1$. The other limit $\mu = 0$ MeV corresponds to the polynomial fit. The variation with the parameter μ is taken as uncertainties in the chiral extrapolation within this model. This shows that the value obtained with the polynomial fit ($\mu = 0$ MeV), 147(3) MeV (here the errors are statistical only), may be affected by a "hidden" chiral logarithm, leading to 128(2) MeV if the effect is maximal ($\mu = \infty$ MeV).

A similar analysis can be made for the heavy-light decay constant we have discussed above. The fits are shown in Fig. 1 for $\mu = 300$ and 500 MeV (thin dotted curves) as well as for ∞ MeV (dashed curve). The effect of the chiral logarithm can be -11% for f_B, if we take $\mu = \infty$ as an extreme case. While this case is probably unrealistic, as it implies the validity of ChPT at very large mass scales, we take this as a conservative estimate of the systematic error, giving the lower limit for f_B. Other functional forms may also be adopted (see, e.g., [20]), but such models are expected to give numerically similar results in so far as the model is constrained by lattice data in the heavy pion mass region and by ChPT in the light pion mass region.

The effect of the chiral logarithm is small for f_{B_s}, since the particle circulating the loop is kaon or eta. The formula in the partially quenched QCD is given in [21]. The chiral extrapolation is shown in Fig. 1 with the lines for two extreme cases $\mu = 0$ and ∞ MeV. The difference between the two is only 1%.

To quote our results we take the central value from the polynomial fit and include the variation in the presence of the chiral logarithm as an error. We obtain

$$f_{B_d} = 191(10)(^{+0}_{-19})(12)(-)\ \text{MeV}, \tag{2}$$

$$f_{B_s} = 215(9)(^{+0}_{-2})(13)(^{+6}_{-0})\ \text{MeV}, \tag{3}$$

$$\frac{f_{B_s}}{f_{B_d}} = 1.13(3)(^{+12}_{-0})(2)(^{+3}_{-0}), \tag{4}$$

where the first error is statistical, the second is the uncertainty from the chiral extrapolation, and the other two are systematic errors explained in what follows. The error from the chiral extrapolation is one sided, since the polynomial fit is taken as our central value. The systematic error given in the third parenthesis is those arising from the finite lattice spacing (truncation of the actions and currents, and their perturbative matching) and the truncation of terms higher order in $1/m_Q$ in the NRQCD action. An order estimate of the truncation errors shows that the most important contributions are $O(\Lambda_{\text{QCD}}^2/m_b^2) \sim 4\%$ and $O(\alpha_s^2) \sim 4\%$. We add these errors by quadratures together with other possible errors. In [10], it is shown for the quenched lattice that such estimates correctly describe the error of finite lattice spacing (see also [11] for B_B). The errors we obtained are consistent with those in the quenched case at the comparable lattice spacing. The errors in the last parenthesis represent the ambiguity in the determination of the strange quark mass, for which we adopt the value with the K mass as the central value.

For the B parameter, ChPT predicts $-(1 - 3g^2)/2$ for the coefficient of the chiral log term instead of $3(1 + 3g^2)/4$ in (1) [21]. Therefore, the effect of the chiral logarithm is negligible in practice. For B_{B_s} there is no chiral logarithm as a function of sea quark mass.

Figure 3 shows the chiral extrapolation of $B_{B_q}(\mu_b)$ at $\mu_b = m_b$ ($= 4.8$ GeV) and the fits without the chiral logarithm. The triangles show the quenched results. The sea quark effect is small for this quantity.

Our unquenched results obtained with a linear chiral extrapolation are

$$B_{B_d}(m_b) = 0.836(27)(^{+0}_{-27})(56)(-), \tag{5}$$

$$B_{B_s}(m_b) = 0.850(22)(^{+18}_{-0})(57)(^{+5}_{-0}), \tag{6}$$

$$\frac{B_{B_s}}{B_{B_d}} = 1.017(16)(^{+53}_{-0})(17)(^{+6}_{-0}). \tag{7}$$

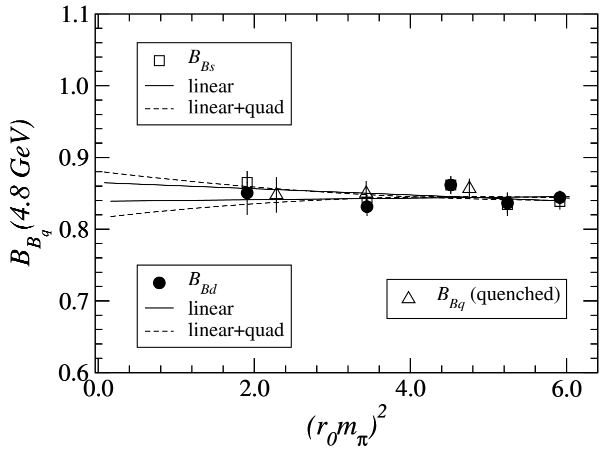

FIG. 3. Chiral extrapolation of B_{B_d} (filled circle) and B_{B_s} (open square). The four-quark operator is perturbatively renormalized, and the "method I" is employed for the truncation of higher order corrections (in α_s and $1/m_b$) as an example [11].

The meaning of errors is the same as for f_B, except for the second one, i.e., those associated with the chiral extrapolation: we take the central value from the linear fit and put the difference from the linear plus quadratic fit as the systematic error.

The amplitude of neutral B meson mixing is proportional to $f_B^2 B_B$. Using the conventionally adopted renormalization-scale independent definition $\hat{B}_B$, which is related to $B_B(m_b)$ as $\hat{B}_B = 1.528 B_B(m_b)$ for $\Lambda^{(5)}_{\overline{\rm MS}} =$ 225 MeV, we find

$$f_{B_d}\sqrt{\hat{B}_{B_d}} = 215(11)(^{+0}_{-23})(15)(-)\ \mathrm{MeV}, \tag{8}$$

$$f_{B_s}\sqrt{\hat{B}_{B_s}} = 245(10)(^{+3}_{-2})(17)(^{+7}_{-0})\ \mathrm{MeV}, \tag{9}$$

and for the SU(3) breaking ratio ξ,

$$\xi = 1.14(3)(^{+13}_{-0})(2)(^{+3}_{-0}). \tag{10}$$

The chiral extrapolation gives the largest entry of systematic errors for ξ, as also suggested in [22]. Compared to the commonly assumed number in the phenomenological analysis, $f_{B_d}\sqrt{\hat{B}_{B_d}} = 230(28)(28)$ MeV (e.g., [23]), where the second error is the quenching uncertainty, our central value of (8) is slightly lower and the quenching error is eliminated.

In conclusion we have obtained an unquenched lattice estimate of the B^0-$\bar{B}^0$ mixing matrix elements, including the decay constant, in a consistent set of simulations. Although the simulation is made at a relatively large mass of dynamical quarks, we explored the range of errors associated with the chiral extrapolation: we expect that the true values of the matrix elements are within the range of indicated errors, even if the chiral logarithm would become manifest at a small quark mass.

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