$B \to \pi ll$ Form Factors for New Physics Searches from Lattice QCD

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The rare decay $B \to \pi\ell^+\ell^-$ arises from $b \to d$ flavor-changing neutral currents and could be sensitive to physics beyond the standard model. Here, we present the first *ab initio* QCD calculation of the $B \to \pi$ tensor form factor f_T. Together with the vector and scalar form factors f_+ and f_0 from our companion work [J. A. Bailey *et al.*, Phys. Rev. D 92, 014024 (2015)], these parametrize the hadronic contribution to $B \to \pi$ semileptonic decays in any extension of the standard model. We obtain the total branching ratio $\mathrm{BR}(B^+ \to \pi^+\mu^+\mu^-) = 20.4(2.1) \times 10^{-9}$ in the standard model, which is the most precise theoretical determination to date, and agrees with the recent measurement from the LHCb experiment [R. Aaij *et al.*, J. High Energy Phys. 12 (2012) 125].

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Motivation.—Hadron decays that proceed through flavor-changing neutral currents may be sensitive to new physics, because their leading standard model contributions are loop suppressed. Here we study the semileptonic decay $B \to \pi\ell^+\ell^-$, which proceeds through a $b \to d$ transition. Hadronic effects in this decay are parametrized by three form factors. In this Letter, we present the first *ab initio* QCD calculation of the tensor form factor f_T, based on lattice-QCD work that also yielded the vector and scalar form factors, f_+ and f_0 [1]. Lattice QCD has several advantages over other approaches to the form factors [2–9], particularly in providing a path to controlled uncertainties that can be systematically reduced [10].

The LHCb experiment recently made the first observation of $B^+ \to \pi^+\mu^+\mu^-$ [11], while the B factories have set limits on the e^+e^- and $\tau^+\tau^-$ channels [12–14]. Below we present the first calculations of $B \to \pi\ell^+\ell^-$ ($\ell = e, \mu, \tau$) observables in the standard model using form factors with fully controlled uncertainties.

The form factors f_+, f_0, and f_T suffice to parameterize $B \to \pi$ decays in all extensions of the standard model. New physics from heavy particles—such as those appearing in models with supersymmetry [3,15–17], a fourth generation [18], or extended [15,19–23] or composite [24] Higgs sectors—alter Wilson coefficients in the effective Hamiltonian pertaining to particle physics below the electroweak scale [25–28]. Whatever these unknown particles may be, the hadronic physics remains the same.

Lattice-QCD calculation.—Our work on $f_T(q^2)$ was carried out in parallel with $f_+(q^2)$ and $f_0(q^2)$. Our aim in Ref. [1] was a precise determination of the Cabibbo-Kobayashi-Maskawa (CKM) element $|V_{ub}|$, and every step of the analysis was subjected to many tests. Further, two of the authors applied a multiplicative offset to the numerical data at an early stage. This “blinding” factor was disclosed to the others only after finalizing the error analysis. Full details of the simulation parameters, analysis, and cross-checks are given in Ref. [1].

Our calculation uses ensembles of lattice gauge-field configurations [29] from the MILC Collaboration [30–32], which are generated with a sea of up, down, and strange quarks. In practice, the up and down sea quarks have the same mass, and the strange-quark mass is tuned close to its physical value. The statistics are high, with 600–2200 gauge-field configurations per ensemble. The physical volume is large enough that we can repeat the calculation in different parts of the lattice, thereby quadrupling the statistics. We use four lattice spacings ranging from 0.12 to 0.045 fm to control the extrapolation to zero lattice spacing.

The tensor form factor is defined via the matrix element of the $b \to d$ tensor current $i\bar{d}\sigma^{\mu\nu}b$:

$$\langle \pi(p_\pi)|i\bar{d}\sigma^{\mu\nu}b|B(p_B)\rangle = 2\frac{p_B^\mu p_\pi^\nu - p_B^\nu p_\pi^\mu}{M_B + M_\pi} f_T(q^2), \qquad (1)$$

where p_B and p_π are the particles' momenta and $q = p_B - p_\pi$ is the momentum carried off by the leptons. The Lorentz invariant q^2 is related to the pion energy in the B-meson rest frame via $E_\pi = (M_B^2 + M_\pi^2 - q^2)/2M_B$. In the finite volume that can be simulated on a computer, E_π takes discrete values, dictated by the spatial momenta $\boldsymbol{p}_\pi$ compatible with periodic boundary conditions. Because statistical and discretization errors increase with pion momentum, we restrict $|\boldsymbol{p}_\pi| \le |2\pi(1,1,1)/L|$. The resulting simulation range of $E_\pi \lesssim 1$ GeV is significantly smaller than the kinematically allowed range of $E_\pi \le 2.5$ GeV. Extending this discrete set of calculations into the full q^2 dependence is the central challenge of this work, and is met in two steps.

The two light quarks (up and down) have a mass larger than it should be, but the range simulated is wide and the smallest pion mass is 175 MeV, close to nature's 140 MeV. Therefore, we can apply an effective field theory of pions—chiral perturbation theory—to extrapolate the simulation data to the physical point. We use a form of chiral perturbation theory adapted to lattice QCD, with additional terms describing the lattice-spacing dependence [33,34] and with modifications needed for energetic final-state pions [35]. As discussed in Ref. [1], we try several fit variations. For example, we replace the loop integrals with momentum sums appropriate to the finite volume, finding negligible changes in the results. Our final fit includes next-to-next-to-next-to-leading order analytic terms and terms to model the discretization errors of the heavy quark. The latter come from an effective field theory for heavy b quarks [36–38].

Figure 1 shows the q^2 dependence of the errors after the chiral-continuum extrapolation just described. Table I gives a numerical error budget for $f_T(q^2 = 20\ \mathrm{GeV}^2)$. The largest uncertainty comes from the statistical errors, as increased during the chiral-continuum extrapolation. This error is under good control for q^2 corresponding to the spatial momenta that we simulate, but grows large elsewhere.

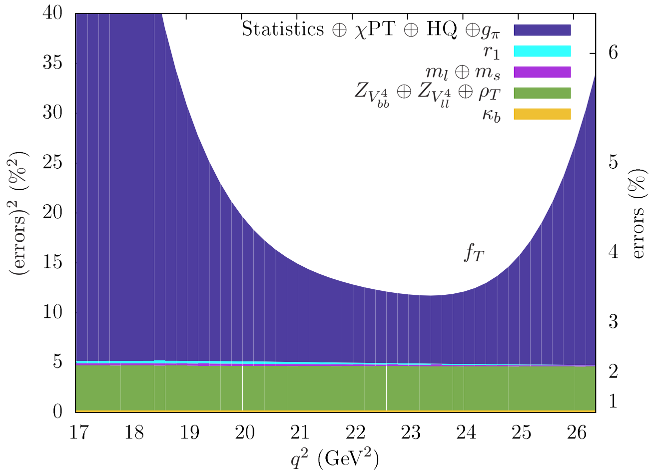

FIG. 1 (color online). Error budget for f_T as a function of q^2 for the range of simulated lattice momenta. The filled bands show the relative size of each error contribution to the total. The quadrature sum is shown on the left y axis and the error itself, in percent, on the right.

The subdominant errors are as follows: To convert from lattice units to physical units, we introduce a physical distance r_1, which is defined via the force between static quarks [39,40]. We use it to form physical, dimensionless quantities, which are the input data for the chiral-continuum fit. At the end, we set $r_1 = 0.3117 \pm 0.0022$ fm [41] based on a related lattice-QCD calculation of $r_1 f_\pi$ [42] and the pion decay constant $f_\pi = 130.41$ MeV [43]. To propagate the parametric uncertainty in r_1 to f_T, we repeat the fit shifting r_1 by $\pm 1\sigma_{r_1}$, leading to the second line in Table I.

In lattice gauge theory, the tensor current does not have the normalization used in QCD phenomenology. We obtain most of the normalization nonperturbatively [44] from $b \to b$ and $d \to d$ transitions with the vector current, with statistical errors below 1%. Another matching factor ρ_T remains, but, by design and in practice, it is close to unity.

TABLE I. Error budget in percent for $f_T(q^2 = 20\ \mathrm{GeV}^2)$. The first error incorporates statistical errors from the simulation and systematics associated with the chiral-continuum fit. The last column emphasizes how the error varies with q^2.

Source of error	δf_T	q^2 dependence
Statistics $\oplus$ χPT $\oplus$ HQ $\oplus$ g_π	3.8	important
Scale r_1	0.5	negligible
Nonperturbative matching $Z_{V^4_{bb}}, Z_{V^4_{ll}}$	0.7	negligible
Perturbative matching ρ_T	2.0	none
Heavy-quark mass tuning κ_b	0.4	none
Light-quark mass tuning m_l, m_s	0.5	negligible
Total (*Quadrature sum of above*)	4.4	important

We calculate ρ_T at the renormalization scale $\mu = m_{b,\mathrm{pole}}$ through first order in the QCD coupling α_s. We estimate the resulting error of order α_s^2 after removing a logarithmic dependence on the matching scale μ, which is present in continuum QCD too. We then examine how the one-loop coefficient depends on heavy-quark mass, identifying the largest value, $\rho_{T,\max}^{[1]}$. Finally, we estimate the error in ρ_T to be $2\alpha_s^2|\rho_{T,\max}^{[1]}|$, evaluating α_s on the second-finest lattice with $a \approx 0.06$ fm. This yields the 2% perturbative-matching uncertainty in Table I.

The last two uncertainties arise as follows. When generating data, we choose the simulation quark masses based on short runs and previous experience. The full analysis yields better estimates. To correct the simulation b-quark mass *a posteriori*, we recompute f_T on one ensemble with two additional values of the bare b-quark mass. Using the slope from all three mass values, we interpolate the data for f_T slightly from the production b-quark mass to the physical value. This leaves an error due to the uncertainty in the size of the b-quark mass correction. The details for f_T are nearly identical to those for f_+ [1], leading to the same estimate, 0.4%, for this error. The light-quark mass dependence is embedded in the chiral-continuum extrapolation, described above. The parametric uncertainty from the input light-quark mass [32] is propagated to f_T by repeating the fit with $\pm 1\sigma_{m_q}$ shifts to these parameters, and is given in the penultimate line of Table I.

The final line in Table I and the upper edge of the stack in Fig. 1 represent the quadrature sum of the systematic uncertainties with the chiral-continuum fit error.

Extension to all q^2.—To extend f_T in the chiral-continuum limit from the range of simulated lattice momenta to the full kinematic range, $0 < q^2 \leq (M_B - M_\pi)^2$, with controlled errors, we use a method based on the analytic structure of the form factor.

In the complex q^2 plane, $f_T(q^2)$ has a cut for timelike $q^2 \geq t_+ \equiv (M_B + M_\pi)^2$ and a pole at $q^2 = M_{B^*}^2$ but is analytic elsewhere. The variable

$$z(q^2, t_0) = \frac{\sqrt{t_+ - q^2} - \sqrt{t_+ - t_0}}{\sqrt{t_+ - q^2} + \sqrt{t_+ - t_0}} \tag{2}$$

maps the whole q^2 plane into the unit disk, with the cut mapped to the boundary and the semileptonic region mapped to an interval on the real axis. Unitarity bounds then guarantee that an expansion of f_T in z (with the B^* pole removed) converges for $|z| < 1$ [45–48]. Following Bourrely, Caprini, and Lellouch (BCL) [49], we factor out the B^* pole and expand in z,

$$(1 - q^2/M_{B^*}^2) f_T(z) = \sum_{n=0}^{N_z - 1} b_n^T \left[z^n - (-1)^{n-N_z} \frac{n}{N_z} z^{N_z} \right], \tag{3}$$

TABLE II. Best-fit values b_n with total errors and correlation matrix ρ_{nm} of the $N_z = 4$ BCL z expansion of f_T. The lower two panels show correlations with the f_+ and f_0 coefficients in Table XIV of Ref. [1] obtained from *ab initio* QCD.

Fit:	0.393(17)	−0.65(23)	−0.6(1.5)	0.1(2.8)
ρ	b_0^T	b_1^T	b_2^T	b_3^T
b_0^T	1.000	0.400	0.204	0.166
b_1^T		1.000	0.862	0.806
b_2^T			1.000	0.989
b_3^T				1.000
b_0^+	0.638	0.321	0.123	0.084
b_1^+	0.321	0.397	0.162	0.109
b_2^+	0.114	0.202	0.198	0.179
b_3^+	0.070	0.152	0.192	0.180
b_0^0	0.331	0.136	0.089	0.073
b_1^0	0.203	0.313	0.198	0.162
b_2^0	0.204	0.268	0.186	0.155
b_3^0	0.151	0.203	0.169	0.149

choosing $t_0 = (M_B + M_\pi)(\sqrt{M_B} - \sqrt{M_\pi})^2$ to minimize $|z|$ in the semileptonic region. Although Eq. (3) was derived for the vector form factor f_+, we use it for the tensor form factor f_T because the two form factors are proportional to each other at leading order in the $1/m_b$ expansion.

We determine the b_n^T with a functional method connecting the independent functions of the chiral-continuum fit with the first several powers of z [1]. Our preferred fit uses $N_z = 4$; adding higher-order terms in z does not significantly change the central value. Table II presents our final result for f_T as coefficients of the $N_z = 4$ BCL z fit and the correlation matrix between them, where the errors include statistical and all systematic uncertainties. This information can be used to reconstruct $f_T(q^2)$ over the full kinematic range. Table II also provides the (mostly statistical) correlations between f_T, f_+, and f_0. Figure 2 shows the extrapolation of f_T to $q^2 = 0$. Table II and Fig. 2 represent the first main result of this Letter.

Implications.—The largest contribution in the standard model to the amplitude for $B \to \pi \ell^+ \ell^-$ is proportional to

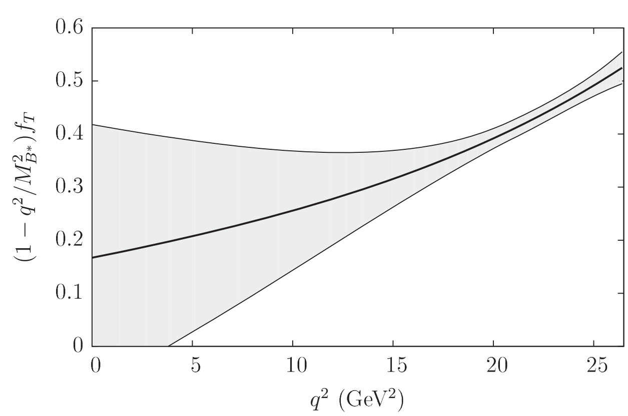

FIG. 2. *Ab initio* result for $f_T(q^2)$ from lattice QCD.

TABLE III. Correlations between BCL coefficients for f_T with those for f_+ and f_0 from Table XIX of Ref. [1], which include experimental shape information from $B \to \pi\ell\nu$ decay.

ρ	b_0^T	b_1^T	b_2^T	b_3^T
b_0^+	0.514	0.140	0.078	0.065
b_1^+	0.111	0.221	−0.010	−0.049
b_2^+	−0.271	−0.232	−0.012	0.029
b_3^+	−0.204	−0.215	−0.013	0.023
b_0^0	0.243	−0.015	−0.025	−0.024
b_1^0	0.005	0.134	0.070	0.057
b_2^0	−0.002	−0.034	−0.032	−0.030
b_3^0	−0.044	−0.061	0.005	0.017

the vector form factor. Assuming that new physics does not contribute significantly to the tree-level decay $B \to \pi\ell\nu$, one can use experimental measurements of this process to constrain the shape of $f_+(q^2)$, especially at low q^2. In Ref. [1], we obtain the CKM element $|V_{ub}|$ from a combined z fit to our lattice-QCD results for f_+ and f_0 and measurements of $\tau_B d\Gamma(B \to \pi\ell\nu)/dq^2$ from *BABAR* [50,51] and Belle [52,53]. This joint fit also yields the most precise current determinations of f_+ and f_0. To enable them to be combined with the results for f_T from Table II, Table III provides the correlations between the z-expansion coefficients for all three form factors. The correlations are small, because f_+ contains independent experimental information.

Using f_T from this work and f_+ and f_0 just described, we show the standard model partial branching fractions for $B \to \pi\ell^+\ell^-$ in Fig. 3. Other ingredients are needed besides the form factors. They appear many places throughout the literature, and, for convenience, some of us have collected them into an appendix of Ref. [54]. In brief, we calculate contributions that cannot be parametrized by the form factors with standard methods, employing QCD factorization at low q^2 [55–63] and an operator product expansion (OPE) in powers of $E_\pi/\sqrt{q^2}$ at large q^2 [64–71]. We take the Wilson coefficients from Ref. [27], the CKM elements from Ref. [72], the meson masses and lifetimes from Ref. [43], and the b- and c-quark masses from Ref. [7]; the numerical values for all parametric inputs used are also tabulated in Ref. [54].

Table IV presents numerical predictions for selected q^2 bins. The last error in parentheses contains effects of parametric uncertainties in α_s, m_t, m_b, m_c, of missing power corrections, taking 10% of contributions not directly proportional to the form factors, and of violations of quark-hadron duality, estimated to be 2% at high q^2 [69]. At low q^2, the uncertainty predominantly stems from the form factors, at high q^2, the CKM elements $|V_{td}^* V_{tb}|$ and form factors each contribute similar errors. Figure 3 and Table IV represent the second main result of this Letter.

In the regions $q^2 \lesssim 1\,\mathrm{GeV}^2$ and $6\,\mathrm{GeV}^2 \lesssim q^2 \lesssim 14\,\mathrm{GeV}^2$, $u\bar{u}$ and $c\bar{c}$ resonances dominate the rate. To estimate the

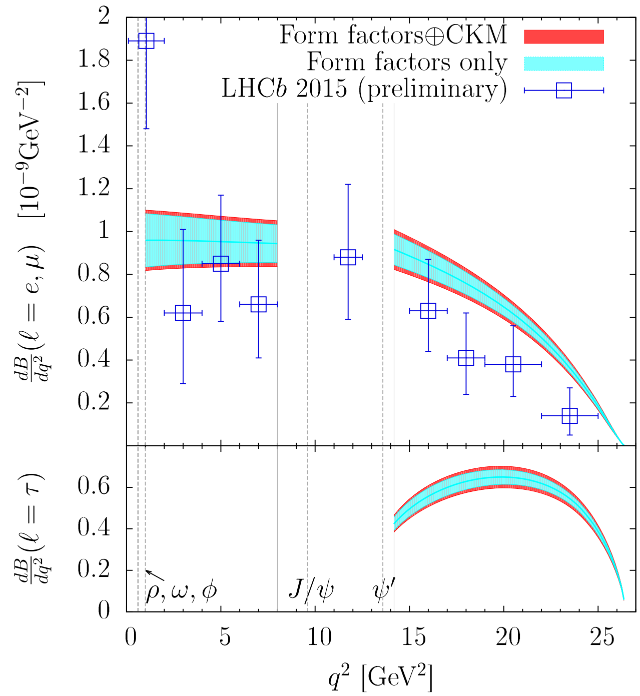

FIG. 3 (color online). Partial branching fractions for $B^+ \to \pi^+\mu^+\mu^-$ (upper panel) and $B^+ \to \pi^+\tau^+\tau^-$ (lower panel) outside the resonance regions. Different patterns (colors) show the contributions from the main sources of uncertainty; those from the remaining sources are too small to be visible. For $B^+ \to \pi^+\mu^+\mu^-$, new measurements from LHCb [73], which were announced after our Letter appeared, are overlaid.

total BR, we simply disregard them and interpolate linearly in q^2 between the QCD-factorization result at $q^2 \approx 8.5\ \mathrm{GeV}^2$ and the OPE result at $q^2 \approx 13\ \mathrm{GeV}^2$. While this treatment does not yield the full branching ratio, it does enable a comparison with LHCb's published result,

TABLE IV. Standard model predictions for $B^+ \to \pi^+\ell^+\ell^-$ partial branching fractions. Those for B^0 decays can be obtained by multiplying by the lifetime ratio $(\tau_{B^0}/\tau_{B^+})/2 = 0.463$. Errors shown are from the CKM elements, form factors, variation of the high and low matching scales, and the quadrature sum of all other contributions, respectively.

$[q^2_{\mathrm{min}}, q^2_{\mathrm{max}}]$ (GeV^2)	$10^9 \times \mathrm{BR}(B^+ \to \pi^+\ell^+\ell^-)$ $\ell = e,\mu$	$\ell = \tau$
[0.1,2.0]	1.81(11,24,6,2)	
[2.0,4.0]	1.92(11,22,6,3)	
[4.0,6.0]	1.91(11,20,6,3)	
[6.0,8.0]	1.89(11,18,5,3)	
[15,17]	1.69(10,13,3,5)	1.11(7,8,2,4)
[17,19]	1.52(9,10,2,4)	1.25(8,8,2,3)
[19,22]	1.84(11,11,3,5)	1.93(12,10,4,5)
[22,25]	1.07(6,6,3,3)	1.59(10,7,4,4)
[1,6]	4.78(29,54,15,6)	
[15,22]	5.05(30,34,7,15)	4.29(26,25,7,12)
$[4m_\ell^2, 26.4]$	20.4(1.2,1.6,0.3,0.5)	

$\mathrm{BR}(B^+ \to \pi^+\mu^+\mu^-) = 23(6) \times 10^{-9}$ [11], which was obtained from a similar interpolation over these regions. Our result $\mathrm{BR}(B^+ \to \pi^+\mu^+\mu^-) = 20.4(2.1) \times 10^{-9}$ agrees with LHCb, and is more precise than the best previous theoretical estimate [7] because we use f_T directly, which avoids a large uncertainty from varying the matching scale μ.

Outlook.—The largest uncertainty in our determination of the $B \to \pi$ form factors is the combined error from statistics with chiral-extrapolation and discretization effects included. We will be able to reduce these with calculations on the MILC Collaboration's recently generated four-flavor ensembles with physical light-quark masses [74]. LHCb's measurement of $\mathrm{BR}(B^+ \to \pi^+\mu^+\mu^-)$ will improve, and Belle II expects to observe the neutral decay mode $B^0 \to \pi^0\ell^+\ell^-$. If a deviation from the standard model is observed, our form factors can be used to compute other observables such as asymmetries, thereby providing information about new heavy particles, such as their masses, spin, and couplings.

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Note added.—Recently, the LHCb experiment announced a new measurement for the $B^+ \to \pi^+\mu^+\mu^-$ differential decay rate [73]. The new results are shown in Fig. 3. The large difference in the lowest q^2 bin is due to the presence of light (ρ, ω, ϕ) resonances, whose effects are important but cannot be estimated in a model-independent manner. Given the present experimental and theoretical uncertainties, it is too early to discern possible new physics contributions to this process.

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