$B \to \pi \ell \ell$ 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 parameterize the hadronic contribution to $B \to \pi$ semileptonic decays in any extension of the Standard Model. We obtain the total branching ratio $\text{BR}(B^+ \to \pi^+ \mu^+ \mu^-) = 20.4(2.1) \times 10^{-9}$ 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., JHEP 1212, 125 (2012)]. Note added: after this paper was submitted for publication, LHCb announced a new measurement of the differential decay rate for this process [T. Tekampe, talk at DPF 2015], which we now compare to the shape and normalization of the Standard-Model prediction.

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Motivation — Hadron decays that proceed through flavor-changing neutral currents may be sensitive to physics beyond the Standard Model, 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 parameterized 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,
Our calculation uses ensembles of lattice gauge-field configurations [29] from the MILC Collaboration [30–32], which are generated with a realistic 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 fm 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 $i\sigma^{\mu\nu}b$:

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

where $p_B$ and $p_\pi$ 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, $E_\pi$ takes discrete values, dictated by the spatial momenta $p_\pi$ compatible with periodic boundary conditions. Because statistical and discretization errors increase with pion momentum, we restrict $|p_\pi| \leq |\pi(1,1,1)/L|$. The resulting simulation range of $E_\pi \lesssim 1$ GeV is significantly smaller than the kinematically allowed range of $E_\pi \leq 2.5$ 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 $f_T(q^2 = 20\text{ GeV}^2)$. 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.

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 $r_1 f_T$ [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 $b \to d$ and $d \to d$ transitions with the vector current, with statistical errors below 1%. Another matching factor $\rho_T$ remains, but, by design and in practice, it is close to unity. We calculate $\rho_T$ at the renormalization scale $\mu = m_{b,pole}$ through first order in the QCD coupling $\alpha_s$. 

### Table I. Error budget in per cent for $f_T(q^2 = 20$ GeV$^2$).

| Source of error | $\delta f_T$ | $q^2$ dependence |
|-----------------|--------------|------------------|
| Statistics $\oplus \chi$PT $\oplus$ HQ $\oplus g_s$ | 3.8 | important |
| Scale $r_1$ | 0.5 | negligible |
| Nonperturbative matching $Z_{V_{tb}}$, $Z_{V_{t\ell}}$ | 0.7 | negligible |
| Perturbative matching $pr_T$ | 2.0 | none |
| Heavy-quark mass tuning $k_b$ | 0.4 | none |
| Light-quark mass tuning $m_l$, $m_s$ | 0.5 | negligible |
| Total (Quadrature sum of above) | 4.4 | important |

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 per cent, on the right.
We estimate the resulting error of order $\alpha_s^2$ after removing a logarithmic dependence on the matching scale $\mu$, which is present in continuum QCD too. We then examine how the one-loop coefficient depends on heavy-quark mass, identifying the largest value, $\rho_{1,\max}$. Finally, we estimate the error in $\rho_T$ to be $2\alpha_s^2(\rho_{1,\max})$, evaluating $\alpha_s$ 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 $f_\pi$ [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.

For 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 $q^2 \geq t_*= (M_B + M_\pi)^2$ and a pole at $q^2 = M_B^2$, but is analytic elsewhere. The variable

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

(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 $z$:

$$(1 - q^2/M_{B^*}^2)f_T(z) = \sum_{n=0}^{N_z-1} b_n^T z^n - (1)^n z^{-N_z} n \frac{N_z}{N_\pi} z^{N_\pi},$$

(3)

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 $f_\pi$, 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 $f_T$, $f_\pi$, 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 $B \rightarrow \pi \ell^+\ell^-$ is proportional to the vector form factor. Assuming that new physics does not contribute significantly to the tree-level

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

| $q^2$ (GeV$^2$) | $f_T(5.2)$ | $f_T(10)$ | $f_T(20)$ |
|----------------|------------|-----------|-----------|
| 0.6            | 0.393(17)  | -0.65(23) | 0.6(1.5)  |
| 1.0            | 0.400      | -0.682    | 0.806     |
| 1.5            | 0.700      | 0.152     | 0.192     |
| 2.0            | 0.638      | 0.321     | 0.123     |
| 2.5            | 0.321      | 0.397     | 0.162     |
| 3.0            | 0.114      | 0.202     | 0.198     |
| 3.5            | 0.070      | 0.152     | 0.192     |
| 4.0            | 0.331      | 0.136     | 0.089     |
| 4.5            | 0.203      | 0.313     | 0.198     |
| 5.0            | 0.204      | 0.268     | 0.186     |
| 5.5            | 0.151      | 0.203     | 0.169     |
| 6.0            | 0.149      |           |           |

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**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.

| \( \rho \) | \( b_0 \) | \( b_1 \) | \( b_2 \) | \( b_3 \) |
|---|---|---|---|---|
| \( b_0 \) | 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 |
| \( b_4 \) | 0.243 | −0.015 | −0.025 | −0.024 |
| \( b_5 \) | 0.005 | 0.134 | 0.070 | 0.057 |
| \( b_6 \) | −0.002 | −0.034 | −0.032 | −0.030 |
| \( b_7 \) | −0.044 | −0.061 | 0.005 | 0.017 |

In the regions \( q^2 \lesssim 1 \) GeV\(^2\) and \( 6 \) GeV\(^2 \lesssim q^2 \lesssim 14 \) GeV\(^2\), \( u\bar{u} \) and \( c\bar{c} \) resonances dominate the rate. To estimate the total BR, we simply disregard them and interpolate linearly in \( q^2 \) between the QCD-factorization result at \( q^2 \approx 8.5 \) GeV\(^2\) and the OPE result at \( q^2 \approx 13 \) GeV\(^2\). While this treatment does not yield the full branching ratio, it does enable a comparison with LHCb’s published result, \( \text{BR}(B^+ \to \pi^+ \mu^+ \mu^-) = 23(6) \times 10^{-9} \) [11], which was obtained from a similar interpolation over these regions. Our result \( \text{BR}(B^+ \to \pi^+ \mu^+ \mu^-) = 20.4(2.1) \times 10^{-9} \) 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 \( \mu \).
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 $\text{BR}(B^+ \to \pi^+ \mu^+ \mu^-)$ 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.

Note added: after this paper was submitted for publication, the LHCb experiment announced a new measurement for the $B^+ \to \pi^+ \mu^+ \mu^-$ differential decay rate [54]. The new results are shown in Fig. 3. The large difference in the lowest $q^2$ bin is due to the presence of light ($\rho, \omega, \phi$) 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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