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A lattice QCD perspective on weak decays of b and c quarks
Snowmass 2022 White Paper

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Lattice quantum chromodynamics has proven to be an indispensable method to determine non-perturbative strong contributions to weak decay processes. In this white paper for the Snowmass community planning process we highlight achievements and future avenues of research for lattice calculations of weak b and c quark decays, and point out how these calculations will help to address the anomalies currently in the spotlight of the particle physics community. With future increases in computational resources and algorithmic improvements, percent level (and below) lattice determinations will play a central role in constraining the standard model or identifying new physics.

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I. INTRODUCTION

Processes involving weak decays of b or c quarks may provide a window on new physics not described by the standard model (SM) of elementary particle physics. For several years such weak decay processes have shown persistent differences of a few standard deviations between theoretical predictions of the SM and experimental measurements. The most prominent deviations, commonly referred to as B anomalies, include

- Ratios testing lepton flavor universality for tree-level decays such as $B \to D^{(*)}\ell\nu$
- Tests of lepton flavor universality for rare, loop-level decays such as $B \to K^{(*)}\ell^+\ell^-$
- Differences in certain q^2 bins/ranges for rare decay differential branching fractions e.g. $B \to K^*\ell^+\ell^-$, $B_s \to \phi\ell^+\ell^-$ and corresponding derived angular observables like P_5'
- Some tension in the branching fraction for the rare leptonic decay $B_s \to \mu^+\mu^-$
- Tension between exclusive and inclusive determinations of CKM matrix elements $|V_{ub}|$ and $|V_{cb}|$

In addition, the use of QCD factorization to describe nonleptonic decays is under scrutiny due to observed large discrepancies with experimental results. Summaries and further details can be found, for example, in [1–3] and in recent reviews of lattice calculations [4–7]. Currently no single quantity is considered significant and trustworthy enough to claim a smoking gun signal for new physics. While deviations in ratios testing lepton flavor universality mostly point in the same direction and collectively favor some SM extensions over others, the tension between exclusive and inclusive determinations of Cabbibo-Kobayashi-Maskawa (CKM) matrix elements lacks a good phenomenological explanation and may hint at underestimated uncertainties. Understanding and resolving the nature of these B anomalies is the challenge for the coming years.

With ongoing and future experimental measurements from Belle II, LHCb, ATLAS, CMS, and BES III, it is critical for theoretical predictions to improve to fully leverage increased experimental precision. A key ingredient here are SM predictions for contributions due to quantum chromodynamics (QCD), which describes the strong interactions of quarks and gluons. Standard perturbative methods work reliably only at (very) high energies and truly nonperturbative concepts are required to study the low energy range. Lattice field theory (LFT) is a nonperturbative framework to study QCD processes at low as well as at high energies. Based on first principles, LFT uses the QCD Lagrangian to simulate the strong interaction using Markov chain Monte Carlo methods. After using a few experimental quantities to fix input values like bare quark masses, many predictions for QCD processes can be calculated and the accuracy of the results can be systematically improved.

Specifically, lattice QCD provides theoretical input that enables us to determine parameters of the SM such as the renormalized quark masses, as well as quantities parametrizing nonperturbative hadronic properties like decay constants, form factors, bag parameters, or the QCD contribution to lifetimes. Precise knowledge of such quantities is essential to enhance our understanding of the SM and distinguish, for example, QCD effects from new physics. In the remainder of this section, we summarize some of the major achievements of and opportunities for lattice QCD for weak b and c decays, and refer the reader to the relevant part of Section II for more details.

In the heavy quark sector, lattice determinations of the leptonic decay constants f_B and f_{B_s} are needed for SM predictions of the rare processes $B \to \mu^+\mu^-$ and $B_s \to \mu^+\mu^-$. Here the lattice community has managed to determine both decay constants to the sub-percent level ($\sim 0.6(0.7)\%$ for $f_B(f_{B_s})$ [4]), so that hadronic uncertainties are now sub-dominant to other sources of error. For $D_{(s)}$ mesons, f_D and f_{D_s} are used to extract $|V_{cd}|$ and $|V_{cs}|$ from leptonic decay measurements. Here also the uncertainties in the decay constants are well below those from experiment. Further progress can be achieved by including quantum electrodynamics (QED) and strong-isospin breaking effects into the lattice calculations, and significant advances have been made in this direction [8–14]. The status and physics impact of heavy meson leptonic decays are expanded on in Section II A.

Semileptonic decay processes are critical inputs for heavy flavor studies, where lattice predictions allow for extraction of CKM matrix elements and give pure SM predictions of R-ratios and other quantities under study. The most precise exclusive determinations of $|V_{ub}|$ and $|V_{cb}|$ come from combining experimental and lattice results for $B \to \pi\ell\nu$ and $B \to D^{(*)}\ell\nu$ respectively. In recent years, LHCb has given first measurements of processes such as $B_c \to J/\psi\ell\nu$, $B_s \to D_s^{(*)}\ell\nu$, $B_s \to K\ell\nu$, and heavy baryon decays. The lattice community has kept pace with theoretical calculations of these same processes. Progress and outlook for this important class of decays is explored in more detail in Section II B.

Meson mixing and lifetimes are discussed in II C. For neutral B-mixing, which is dominated by short-distance operators, lattice QCD has already delivered ratios of mass differences with precision around 1.5%, compared to experimental uncertainties of around 0.4%. The dominant sources of systematic error in the lattice QCD calculations can be reduced or eliminated with modern techniques. The next five years are likely to see high-precision calculations of both bag parameters ($< 1\%$) and for ratios ($< 0.5\%$), bringing results to point where QED effects become important. Neutral D-meson mixing presents a greater challenge both experimentally and theoretically. The short-distance, CP-violating ($\Delta C = 2$) matrix elements have already been determined via lattice QCD with roughly 5% statistical precision, comparable to experimental measurements.

Quark masses – fundamental parameters of the SM important for high precision tests of the Higgs sector – have achieved an impressive level of precision ($\lesssim 1.0(0.5)\%$ for m_c (m_b) [4]), thanks to long-term efforts from the community. Here also calculations have reached near to the "QED wall" where electromagnetic effects must be accounted for. Details of progress in this area are given in Section II D.

Moving beyond these "traditional" areas, members of the community have continued to innovate and expand the scope of physics accessible to lattice computation. Important examples of this relevant to studies of heavy flavor include first-principles computation of radiative decay processes (Section II E), development and implementation of theoretical machinery to handle multi-hadron states (discussed in Sections II B and II C), and exploration of methods to determine inclusive decay rates, which would be invaluable for resolving inclusive/exclusive discrepancies in determinations of CKM matrix elements (Section II F). Each of these areas herald a significant advance in our ability to calculate strong processes from first principles, and in the relevant subsections we have attempted to provide context on the remaining challenges and potential timeline to make an impact on phenomenology.

We close by briefly touching on the computational aspects needed to pursue the outlined calculations in Sec. III.

II. PROSPECTS AND CHALLENGES

Lattice calculations with charm and bottom quarks face the challenge that in order to keep discretization effects in simulations with fully relativistic actions under control, the quark mass m_q must obey $m_q < a^{-1}$. Here a^{-1} is the inverse lattice spacing or cutoff typically given in [GeV], whereas the lattice spacing a is quoted in [fm]. In the past, but also in certain calculations today, the large mass of charm and especially bottom quarks make it impossible to meet this requirement, forcing the use of effective actions. By now algorithmic improvements and increased computational power enable the use of a fully relativistic setup for all quarks and more fully relativistic calculations will be published in the near future. A fully relativistic setup features a simpler and more accurate handling of the renormalization, which for most calculations will be performed nonperturbatively. By combining simulations either featuring up/down quarks at their physical mass or close-to-physical mass bottom quarks, we can already today largely eliminate two major sources of uncertainty: chiral extrapolation and the need for (partly) perturbative renormalization schemes at low energies. By further decreasing the lattice spacing to $a \le 0.044\,\mathrm{fm}$ ($a^{-1} \gtrsim 4.5\,\mathrm{GeV}$), even bottom quarks can be simulated with the same action as up/down quarks. With further improved numerical performance, fully dynamical simulations with up/down, strange, charm, and bottom quarks become possible [15], although a practical improvement due to simulating dynamical bottom quarks is most likely marginal. In addition machine learning techniques may offer new possibilities for LFT [16]. Complementary to LFT calculations would be to directly perform quantum simulations [17]. That however requires to have quantum computers with (very) many qubits and long enough coherence time.

A. Leptonic decays

Determinations of leptonic decay constants for $D_{(s)}$ [18–36], $B_{(s)}$ [22, 23, 26, 32, 35, 37–46], and B_c [47, 48] mesons, obtained from 2-point lattice correlation functions at zero momentum, showcase the potential of lattice QCD calculations. Several groups have determined decay constants with high precision and a complete error budget. The agreement between the different results strengthens the credibility of lattice results overall and leads to even more precise average values presented by the Flavor Lattice Averaging Group (FLAG) [4]. Using the lattice averages for f_D, f_{D_s}, and f_B, together with available experimental data for the corresponding leptonic decays, provides a way of extracting the CKM matrix elements $|V_{cd}|$, $|V_{cs}|$, and $|V_{ub}|$, respectively. For all three cases lattice QCD uncertainties are well below those of experiment.

The most precise determinations of $|V_{cd}|$ at present come from combining experimental measurements of $D \to \ell\nu_\ell$ with the lattice determinations of f_D. Until last year, the most precise values of $|V_{cs}|$ similarly came from $D_s \to \ell\nu_\ell$ and f_{D_s}, but new lattice results for the semileptonic decay $D \to K\ell\nu$ [49] are improving on this (see Section II B). The leptonic determination of $|V_{ub}|$ is not competitive with that from semileptonic decays, but with improvements in the experimental precision expected from Belle II, it could help to shed light over the inclusive-exclusive tension in the determination of that parameter.

With precision around or below the percent level, future progress to reduce uncertainties will require electromagnetic and strong isospin breaking effects be accounted for. Lattice calculations combining QED and QCD in the heavy quark sector have already been demonstrated e.g. in the case of charmonium [50] and bottomonium [51]. Further details on radiative decays, which lift helicity suppression, and radiative corrections are presented in Sec. II E.

Lattice determinations of neutral B meson decay constants are also crucial inputs for the study of rare leptonic decays. These flavor-changing neutral current (FCNC) processes are highly suppressed in the SM, and provide important constraints on new physics. They are largely determined by the same QCD matrix elements as the decay constants, with corrections from subleading operators. The branching ratio for $B_s \to \mu^+\mu^-$ is rather precisely determined [52–54] using the lattice input for f_{B_s}, and shows some tension with the current experimental result [55–57]. For $B_d \to \mu^+\mu^-$, the theory error is larger [52, 53], but the result is consistent with the less well-determined experimental value [56, 57]. Similarly to the extraction of CKM matrix elements, in these comparisons lattice QCD inputs have now exceeded the precision of corresponding experimental measurements. Further insight on the above theory-experiment tension could be extracted from a correlated analysis with the parameters that describe $B_{(s)}$ meson mixing [58].

B. Exclusive semileptonic decays at tree- and loop-level

Semileptonic decays provide a rich variety of hadronic systems to study many different decay processes, extract CKM matrix elements, and perform stringent tests on the SM. To extract CKM matrix elements, experimental results for tree-level branching fractions are combined with form factors calculated using lattice QCD. These combinations often provide the most precise determinations of the relevant CKM matrix elements, as for $|V_{cs}^{\text{excl.}}|$, $|V_{ub}^{\text{excl.}}|$, or $|V_{cb}^{\text{excl.}}|$ [4]. Both tree-level weak charged current and loop-suppressed flavor-changing neutral current (FCNC) semileptonic decays provide tests of the SM via comparison of experimental measurements and SM predictions for differential rates, angular distributions, or ratios of decays with the same hadronic final state but different generations of final-state leptons. These ratios test lepton flavor univerality (LFU) and have received substantial attention due to few-σ tensions between experiment and theoretical predictions for several decay channels. Several experiments have reported such ratios for tree-level decays (e.g. $B \to D^{(*)}\ell\nu$ [59–62] or $B_c \to J/\psi\ell\nu$ [63]) as well as rare loop-level $b \to \{s,d\}\ell\ell$ decays (e.g. $B \to K^{(*)}\ell^+\ell^-$ [64–69] or $B_s \to \phi\ell^+\ell^-$ [70, 71]) including also baryonic initial and final states ($\Lambda_b^0 \to pK^-\ell^+\ell^-$ [72] or $\Lambda_b^0 \to \Lambda_c^+\tau^-\bar{\nu}_\tau$ [73]). On the theory side, these ratios are exceptionally clean, and reported tensions with experimental observations have increased interest in those quantites. While tensions vary for different processes, it is intriguing that these can be accounted for in a model-independent way by assuming new-physics contributions to certain Wilson coefficients of the effective weak Hamiltonian. For details see, e.g., Refs. [74–79] as well as references within. Global fits to $b \to s\ell\ell$ and $b \to c\ell\nu$ anomalies provide a basis to build new physics models. Candidates include, for instance, scenarios with a Z' boson [80–83], leptoquarks [84–93], or scenarios related to supersymmetry (SUSY) [94–96]. For an overview and further details see Ref. [97].

To help confirm or refute the observed deviations, higher-precision calculations of semileptonic form factors are needed, with systematic and statistical uncertainties commensurate with current and upcoming experiments. From the perspective of lattice QCD, the simplest processes to compute are semileptonic decays with a pseudoscalar final state. These calculations involve two-point and three-point correlation functions at zero and non-zero momenta, which furnish the two form factors f_+ and f_0 entering at tree-level or also f_T for rare loop-level decays. Calculations exist in the literature for a variety of semileptonic B decays: $B \to \pi\ell\nu$ [98–102], $B \to \pi\ell^+\ell^-$ [103], $B \to K\ell^+\ell^-$ [104, 105], $B_s \to K\ell\nu$ [100, 106–110], $B \to D\ell\nu$ [111–113], $B_s \to D_s\ell\nu$ [108, 110, 113–116] and also for semileptonic D decays: $D \to \pi\ell\nu$ [117–120], $D \to K\ell\nu$ [49, 117, 119–121]. Once the lattice form factors over the full q^2 range have been obtained, it is a simple post-processing task to integrate these form factors over the full q^2 range to obtain R-ratios testing LFU. Hence R-ratios have also been determined for processes like $B \to \pi\ell\nu$ which so far have not been reported by experiments. The extraction of $|V_{ub}^{\text{excl.}}|$ from $B \to \pi\ell\nu$, the most precise channel for that CKM parameter, has commensurate errors coming from experiment and lattice QCD form factors [4]. For $B \to D\ell\nu$ and the extraction of $|V_{cb}^{\text{excl.}}|$, experimental uncertainty presently exceeds the theoretical error from lattice QCD [4]. However, improved theoretical precision will be crucial in both modes in order to make full use of expected improvements in experimental data from Belle II. Improved precision will also be valuable for understanding the inclusive-exclusive tensions for $|V_{ub}|$ and $|V_{cb}|$. Furthermore, LHCb demonstrated its capabilities to determine the ratio $|V_{ub}^{\text{excl.}}/V_{cb}^{\text{excl.}}|$ by performing a combined analysis of $B_s \to K\mu\nu$ and $B_s \to D_s\mu\nu$ [122]. With more statistics and a finer resolution of the q^2 bins this approach can be an interesting alternative to determine the ratio of CKM matrix elements.

In particular, the large mass of the $B_{(s)}$ meson in the initial state leads to a large allowed range of momentum transfer q^2 to the outgoing leptons. Maintaining statistical control, especially at low q^2, presents a challenge for these calculations. A common approach in the literature has been to focus on the high-q^2 behavior and then extend the calculation to full kinematic range using the z-expansion [123–126]. Recent work has revived old ideas about using dispersive bounds [127–131] to constrain the low-q^2 behavior of the form factors given results at high q^2. Even though covering the full q^2 range is computationally challenging, comparing the shape of the form factors to the experimental data across q^2 provides further insight on the quality of our theoretical description of the experimental process. Thanks to the advances in simulating heavy flavors and due to new ensembles with finer lattice spacings, the range of directly accessible q^2 values is increasing. For more than a decade, the full kinematic range has been accessible to lattice QCD calculations of D semileptonic decays. For heavy-to-heavy decays there has been recent progress towards the full q^2 range: $B_s \to D_s \ell\nu$ [115] as well as $B_c \to B_{s,d}$ [132], $B_c \to D^0 \ell\nu$ and $B_c \to D_s \ell^+\ell^-$ [133]. Near-term progress on extending the q^2 range in lattice QCD calculations of B semileptonic decays (especially B-to-light decays) will be key to improved determinations of CKM matrix elements and more stringent tests of the SM.

Exclusive semileptonic decays with vector final states are more challenging and for many years lattice results for heavy-to-heavy transitions were available only at zero recoil ($B \to D^*\ell\nu$ [134, 135] and $B_s \to D_s^*\ell\nu$ [116, 135]). Recently, the first lattice calculation of the form factors for $B \to D^*\ell\nu$ going beyond zero recoil was performed in Ref. [136]. These results gave the first pure-lattice calculation of the LFU ratio $R(D^*)$. Two additional and entirely independent determinations of $B \to D^*\ell\nu$ form factors at non-zero recoil are expected soon [137, 138]. Experimentally $B \to D^*\ell\nu$ is the preferred channel to extract $|V_{cb}^{\text{excl.}}|$. Hence the lattice form factor data for $B \to D^*\ell\nu$ beyond zero recoil are critical to shed light on the tension between exclusive and inclusive determinations of $|V_{cb}|$, compare shapes of the form factors, and test the different methods to constrain the low-q^2 range using more precise data at high q^2. Improved knowledge of the $B \to D^*\ell\nu$ form factors will also benefit the theory prediction of $R(D^*)$, which presently is in tension with the experimental value [139]. Recent results for tree-level decays with vector final states, $B_s \to D_s^*\ell\nu$ [140] and $B_c \to J/\psi\ell\nu$ [141], include all four form factors and directly cover most of the physically allowed q^2 range. Both modes provide alternative ways to extract $|V_{cb}^{\text{excl.}}|$ and may provide useful insight into the theory-experiment tensions for $R(D)$ and $R(D^*)$, especially given expected experimental results from Belle II and LHCb. One outstanding challenge for the future is including the final state's decay width as part of the nonperturbative calculation. For all three processes described above, the vector final-state particle has a very narrow width and can be treated with chiral perturbation theory extended to heavy mesons, or taken to be QCD-stable. However, the target precision dictated by forthcoming experimental data will eventually require a more rigorous treatment, especially for the decay to K^*.

The general formalism enabling lattice studies of $1 \to 2$ hadronic processes, like $B \to K^*(\to K\pi)\ell^+\ell^-$, has been developed in Refs. [142–151]. The formalism provides a rigorous non-perturbative relation between finite-volume Euclidean quantities calculable in lattice QCD and the physical, infinite-volume $1 \to 2$ decay amplitude. Compared to form factor calculations with single-hadron final states, $1 \to 2$ hadronic processes require conceptually different calculations and substantially larger computational effort. For a detailed discussion see Refs. [1, 2] and references therein. While such calculations have already been performed in the light sector, e.g., for $K \to \pi\pi$ [152–156], decays of $B_{(s)}$ and $D_{(s)}$ mesons are typically more challenging because the large decaying meson mass makes additional final states kinematically allowed. The level of difficulty is mainly determined by the energy of the two-hadron final state, so semi-leptonic calculations in which the leptons carry away much of the initial energy are more accessible. In particular, processes such as $B \to K^*(\to K\pi)\ell^+\ell^-$ [150] and $B \to \rho(\to \pi\pi)\ell\nu$ are natural starting points for multi-hadron heavy-flavor decays. Progress in calculating the $K\pi \to K\pi$ scattering amplitude, a required input for the weak decay into this final state, is reported e.g. in Refs. [157, 158].

The kinematics of purely hadronic heavy-flavor decays presents additional challenges. However, by working with an unphysical setup (e.g. heavier-than-physical u/d quarks or lighter-than-physical b/c quarks) the number of kinematically allowed final states can also be controlled in other channels. In this way, the methodology used for calculating $K \to \pi\pi$ can be extended in steps towards $D \to \pi\pi$, for instance. However, honest calculation of the physical process eventually requires a formalism that rigorously treats all important open channels in the decay, including four-particle states. In this vein, work is ongoing to extend the general $1 \to 2$ formalism to more particles. The approach to study weak three-hadron decays, including $K \to \pi\pi\pi$, was recently developed [159, 160].

In the future, this work may open the path to lattice calculations of more advanced phenomenologically interesting processes such as $\overline{B^0} \to D^+\{K^-, \pi^-\}$ [161, 162], or the long distance contribution to neutral D-meson mixing. Long-distance contributions (in the form of charm resonances) also occur in rare loop-level decays such as $B \to K^{(*)}\ell^+\ell^-$ and $B_s \to \phi\ell^+\ell^-$, where typically an operator product expansion (OPE) is used to express matrix elements of nonlocal operators in terms of local-operator matrix elements. In Refs. [163–165] the local matrix elements have been determined on the lattice to extract the seven form factors for $B \to K^*\ell^+\ell^-$ and $B_s \to \phi\ell^+\ell^-$. In this calculation the vector final state is treated as a stable particle, not accounting for the associated systematic uncertainties. Since the observed deviations between theory and experiment for certain q^2 bins have persisted for several years, it is of utmost importance to have well-founded theory predictions. Once again, the kinematics in the light sector is more favorable for lattice calculations, and a proper treatment of long-distance effects in rare kaon decays has been demonstrated [166–172]. Very first steps towards the direct computation of nonlocal matrix elements for $B \to K\ell^+\ell^-$ have been taken in Ref. [173].

In analogy to semileptonic decays of mesons, baryons can decay into a hadronic final state and a lepton pair. While B-factories are mostly run at the $\Upsilon(4s)$ threshold to create $B\bar{B}$-pairs, the experiments at the large hadron collider (LHC) measure decays of any particles originally created from colliding two protons at high energies. LHCb has reported several measurements of semileptonic decays of Λ_b and Λ_c baryons [73, 174–178], while BES III has also reported semileptonic Λ_c decays [179–181]. Belle [182] and ALICE [183] have reported semileptonic Ξ_c decays. Lattice calculations of baryons tend to suffer from a more severe signal-to-noise problem compared to those of mesons [184, 185]. Nevertheless, lattice calculations of baryonic decays have been performed for $\Lambda_c \to n\ell\nu$ and $\Lambda_c \to p\ell^+\ell^-$ [186], $\Lambda_c \to \Lambda\ell\nu$ [187], $\Lambda_c \to \Lambda^*\ell\nu$ [188, 189], $\Lambda_b \to \Lambda_c\tau\bar{\nu}$ [190, 191], $\Lambda_b \to p\ell\bar{\nu}$ [191, 192], $\Lambda_b \to \Lambda\ell^+\ell^-$ [193–196], $\Lambda_b \to \Lambda_c^*\ell\bar{\nu}$ [188, 197], $\Lambda_b \to \Lambda^*\ell^+\ell^-$ [198], and $\Xi_c \to \Xi\ell\nu$ [199]. Integrating the form factors for semileptonic baryon decays over the allowed range of q^2, R-ratios testing lepton flavor universality can be defined and compared to experimental predictions. Likewise CKM matrix elements can be extracted by combining the form factors with experimental data. However, for baryonic decays to enter global averages, additional calculations performed by independent groups are needed [4, 200, 201].

C. Meson mixing and lifetimes

Although a loop-level process, neutral B_s- and B-meson mixing is the preferred experimental channel for extracting the CKM matrix elements $|V_{ts}|$ and $|V_{td}|$. Experiments measure oscillation frequencies with high precision, and global averages [202], dominated by the latest LHCb results [203, 204], show sub-percent level uncertainties. In the SM and beyond, the hadronic contribution to these processes is governed by five local, four-fermion ($\Delta B = 2$) operators. The relevant matrix elements are calculable in lattice QCD via two-point and three-point correlation functions at zero momentum. The SU(3)-breaking ratio ξ [205], formed using the ratio of B_s- and B-meson mixing parameters, is an important input for global CKM unitarity triangle fits [200, 201]. Lattice calculations of ξ have reached percent-level precision [26, 37, 42, 54, 206–209], but further progress is needed to achieve the same level of precision for the matrix elements (expressed, e.g., as "bag parameters") of the individual mixing processes, presently determined at the few percent level. The next five years are likely to see high-precision calculations of both bag parameters ($< 1\%$) and for ratios ($< 0.5\%$), bringing results to point where QED effects become important.

At present, tensions exist among the lattice calculations for some $\Delta B = 2$ operators. Calculations by different groups employ different renormalization schemes, lattice discretizations, and numbers of dynamical quark flavors [26, 37, 42, 54, 208, 210]. Understanding and resolving these tensions is essential for answering the experimental question of whether or not new physics is present in netural B-meson mixing [211–213]. As precision improves, higher dimensional operators of the effective weak Hamiltonian become important, particularly for determination of the lifetime difference $\Delta\Gamma$, which can provide a complementary test for the SM. A pioneering study calculated the dimension-7 operators for neutral meson mixing [214], and confirmation by an independent calculation is desirable.

Neutral D-meson mixing offers complementary constraints on the CKM matrix. Hadronic contributions to this process enter in two classes: short-distance, CP-violating ($\Delta C = 2$) matrix elements and long-distance, CP-preserving ($\Delta C = 1$) matrix elements. The $\Delta C = 2$ matrix elements have already been determined via lattice QCD with roughly $5 - 10\%$ statistical precision [215–217], comparable to experimental measurements. Over the next five years, experimental precision is expected to improve by an order of magnitude [218]. For continued impact, improved lattice calculations are needed on the same timescale. The long-distance $\Delta C = 1$ contributions present a much harder theoretical problem, but the kinematically simpler case of kaon-mixing has been investigated [219–221]. Further development of lattice methods for multi-hadron states will be necessary for direct calculations (see remarks in the previous subsection). Support for ongoing theoretical and algorithmic work is needed to enable controlled lattice QCD calculations of the long-distance $\Delta C = 1$ matrix elements on the ten-year timescale.

B-meson lifetimes are important targets for lattice QCD. Besides the $\Delta B = 2$ operators appearing in mixing, calculations of hadron lifetimes also require $\Delta B = 0$ operators. In particular, lifetime ratios provide valuable tests of expectations from heavy quark effective theory (HQET) (see [222] for a review). While the ratios $\tau(B^+)/\tau(B_s)$ and $\tau(B^0)/\tau(B_s)$ are in good agreement with the HFLAV average [202], the recent ATLAS measurement [223] deviates substantially from recent measurements by LHCb [224, 225] and CMS [226]. To bolster confidence in the theory predictions, currently dominated by QCD sum-rule calculations [211, 227], a state-of-the-art lattice calculation is desirable. Despite early attempts [228–232], no lattice calculation with a complete systematic error budget exists to date. A lattice calculation of lifetimes faces the challenge that operators of different mass dimension mix under renormalization. A breakthrough on that issue could be made by taking advantage of the gradient flow [233–236] and the concept of the short-flow-time expansion [237–240] to define a new, nonperturbative renormalization scheme [241–244]. A further challenge arises from quark-line disconnected contributions, which are notoriously hard to compute with sufficient statistical precision.

D. b and c quark masses

In addition to providing SM predictions of heavy meson and baryon properties, lattice QCD simulations are well-suited to the precision determination of charm and bottom quark masses. These fundamental parameters are needed to stringently test the Higgs sector of the SM [245], by comparing Higgs couplings to b and c quarks measured in experiment with the determinations of quark masses computed via lattice QCD. The precision computation of quark masses has made good progress in recent years [246], with lattice now delivering charm and bottom mass to a (sub-)percent level of precision, laying the groundwork for future experimental tests. Measurements from HL-LHC will be able to pin down coupling to bottom at the few-percent level, and first evidence of coupling to charm may also be achievable [247, 248]. Next generation accelerators could improve these coupling measurements to a level roughly commensurate with present lattice determinations [245, 249].

There are now several different strategies for determining quark mass — among these are approaches based on moments of current-current correlators [250, 251], the implementation of momentum subtraction schemes on the lattice [252, 253], spectroscopy of heavy meson masses and HQET [254, 255], nonperturbative HQET determinations [256] and computations involving step-scaling in small volume [257, 258]. These methods, though all relying crucially on lattice simulation, differ substantially in approach and are hence subject to differing sources of systematic uncertainty. The good agreement amongst results from these approaches [4] gives confidence in the robustness of the determinations at this level of precision. Recently, the effects of adding QED have been quantified, introducing small (but significant at this level of precision) shifts to m_c [50] and m_b/m_c [259]. Moving forward, it will be important to hone the efficacy of existing strategies and also develop new ideas, while the widespread use of multiple techniques will help ensure robust error estimates as values continue to improve.

E. Radiative decays and corrections

The ability to calculate radiative decay processes from first principles is an exciting advance that offers opportunities for precision flavor physics, BSM physics, and hadronic structure. The development of lattice QCD methods to calculate radiative decay processes is relatively recent [8]. The general procedure for the lattice calculations has been demonstrated [11, 14, 260].

The determination of CKM matrix elements from leptonic decays (cf. Sec. II A) at $O(\alpha_{\rm em})$ requires the evaluation of amplitudes with a real photon [8]. Thus, this technology can directly address radiative corrections in leptonic decays and advance lattice calculations beyond the "QED wall" for these important processes. First-principles computations are in progress or planned for the structure-dependent form factors for $B \to \ell\nu_\ell\gamma$, $D_{(s)} \to \ell\nu_\ell\gamma$ and $B_{(s)} \to \ell^+\ell^-\gamma$ and $D_{(s)} \to \ell^+\ell^-\gamma$, with a broad photon energy spectrum [261]. For B decay, an enhancement of the radiative corrections may be expected due to the nearby B^* resonance [262]. Currently only model-dependent predictions of the decay rates are available in the literature based on QCD factorization and sum rules [263–274]. A fully non-factorized, nonperturbative calculation could lead to improved precision in the determination of the corresponding CKM matrix elements.

Adding a hard photon in the final state for leptonic decay of a pseudoscalar meson lifts helicity suppression [275], providing sensitivity to a larger set of operators in the weak effective Hamiltonian. For example the processes $B^0 \to \ell^+\ell^-\gamma$ and $B_s \to \ell^+\ell^-\gamma$ probe additional operators beyond those of the corresponding purely leptonic decays, which can bear on global fits for $b \to s\ell^+\ell^-$, and are well-suited for testing LFU with light leptons [260].

Radiative processes also give important information on hadron structure. For large photon energy the process $B \to \ell\nu_\ell\gamma$ is the cleanest probe of the first inverse moment, $1/\lambda_B$, of the B meson lightcone distribution amplitude, an important input for QCD factorization predictions for nonleptonic B decays [265, 276, 277]. Using the upper limit for $\mathcal{B}(B^- \to \ell^-\bar{\nu}_\ell\gamma, E_\gamma > 1\,\text{GeV})$ from Belle [278] or a lattice form factor calculation can constrain λ_B [279]. A similar calculation in the charm sector would allow to make comparisons with BES III results for $D^+_{(s)} \to e^+\nu_e\gamma$ [280, 281]. An alternate approach, based on recent developments in computing x-dependent hadron structure, may also provide information on the B and D meson distribution amplitudes [282].

F. Inclusive decays

SM predictions for the CKM matrix elements $|V_{ub}|$ and $|V_{cb}|$ have been computed based on both inclusive [202, 283–285] and exclusive [4, 98–100, 134, 136] decay channels. The results have exhibited a long-standing tension, with the size of the tension varying between computations. Compared to their exclusive counterparts, inclusive semileptonic decays present an additional theoretical challenge for lattice QCD. The essential difficulty is extracting Minkowskispace spectral densities from finite-volume Euclidean correlation functions. However, novel and promising ideas [286–290] may have overcome this theoretical hurdle, paving the way for calculations of fully inclusive decay rates from lattice QCD simulations. The new method also opens the door for further applications, such as moments of the lepton energy and the hadronic invariant mass. Exploratory numerical studies now exist [286, 291, 292], raising hopes for future work with physical parameters and controlled systematic uncertainties. These calculations may play a significant role in resolving the tension between inclusive and exclusive determinations of CKM matrix elements. Methods in this entirely new direction in lattice QCD are still in the early stages of development. It is conceivable, however, that results with controlled systematics that are sufficiently precise to allow for meaningful SM tests could become available in the next decade.

III. COMPUTATIONAL RESOURCES

The calculations outlined in this white paper require post-exascale computational resources [293]. A comprehensive research program on weak b and c decays aimed at percent (or subpercent) precision requires gauge-field ensembles where the wavefunctions of both heavy and light degrees of freedom are well resolved and can be studied without distortion. This translates into gauge fields with both small lattice spacings $a \leq 0.044\,\text{fm}$ ($a^{-1} \gtrsim 4.5\,\text{GeV}$) and with large physical volumes $M_\pi \cdot L > 4$. Such simulations require increased lattice sizes. For example, a $256^3 \times 512$ lattice at a lattice spacing $a = 0.040\,\text{fm}$ ($a^{-1} \approx 5\,\text{GeV}$) would allow for simulation of up/down, strange, charm, and bottom quarks at their physical mass in a 10 fm box with $M_\pi \cdot L \approx 7$. Such an ensemble would provide sufficient physical distance between hadronic initial and final states to isolate the required matrix elements in calculations of form factors or meson mixing. Moreover, such large lattices will allow for new analysis concepts based e.g. on masterfields [294]. Simulating all quarks at their physical mass is particularly beneficial for systematic control of calculations like $B \to \rho \ell \nu$, where no effective field theory is available to guide extrapolations to physical masses. The large 10 fm box suppresses finite volume effects, which is especially critical for studying processes with multiple hadrons.

Today, lattice simulations already tackle lattice sizes of $96^3 \times 192$ or $144^3 \times 288$, and research is ongoing to address algorithmic and computational challenges when simulating finer and larger lattices. Due to the algorithmic phenomenon of critical slowing down, development of new alogirithms is likely needed to accelerate sampling the QCD path integral in hadronic systems with multiple length scales. On the computational side, harnessing the rapid increase of computational (GPU) performance is constrained by the stagnating network performance. Communication-suppressing algorithms [295, 296] are promising candidates to meet that challenge and with an anticipated tenfold performance increase with the next generation of machines, a $256^3 \times 512$ lattice could already become viable. Professional software support is essential to ensure that algorithmic advances are leveraged to their full potential (e.g., by using advances in generating gauge field configurations in programs that perform measurment tasks). Post-exascale computing resources, when combined with new and more precise experimental data, will enable tests of the SM in the heavy quark sector with unprecedented precision.

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