Beauty mesons in \( N_f = 2 + 1 + 1 + 1 \) lattice QCD with exact chiral symmetry

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Abstract

We present the first study of \( N_f = 2 + 1 + 1 + 1 \) lattice QCD with domain-wall quarks. The \((b, c, s)\) quarks are physical, while the \((u, d)\) quarks are heavier than their physical masses, with the pion mass \( \sim 700 \text{ MeV} \). The gauge ensemble is generated by hybrid Monte Carlo simulation with the Wilson gauge action for the gluons, and the optimal domain-wall fermion action for the quarks. Using point-to-point quark propagators, we measure the time-correlation functions of quark-antiquark meson interpolators with quark contents \( \bar{b}b, \bar{c}c, \bar{s}s, \) and \( \bar{c}c \), and obtain the masses of the low-lying mesons. They are in good agreement with the experimental values, plus some predictions which have not been observed in experiments. Moreover, we also determine the masses of \((b, c, s)\) quarks.
I. INTRODUCTION

In 2007, we performed the first study of treating valence \((\mathbf{u}, \mathbf{d}, \mathbf{s}, \mathbf{c}, \mathbf{b})\) quarks as Dirac fermions in quenched lattice QCD with exact chiral symmetry \[1, 2\]. The low-lying mass spectra of mesons with quark contents \(\bar{b}b, \bar{b}c, \bar{b}s,\) and \(\bar{c}c\) were determined, together with the pseudoscalar decay constants. Some of our results (e.g., the masses of \(\eta_b\) and \(h_b\)) were theoretical predictions at the time of publication, which turn out to be in good agreement with later experimental results. This asserts that it is feasible to treat \((\mathbf{u}, \mathbf{d}, \mathbf{s}, \mathbf{c}, \mathbf{b})\) valence quarks as Dirac fermions, in lattice QCD with exact chiral symmetry.

Now the question is whether one can simulate dynamical \((\mathbf{u}, \mathbf{d}, \mathbf{s}, \mathbf{c}, \mathbf{b})\) quarks in lattice QCD with exact chiral symmetry. This motivates the present study. Since the \(\mathbf{b}\) quark is heavy, with mass \(m_b \sim 4500\,\text{MeV}/c^2\), it requires a fine lattice spacing such that the condition \(m_ba < 1\) is well satisfied in order to keep the discretization error under control. On the other hand, to keep the finite-volume error of the light hadrons under control, the lattice size \(L\) has to be sufficiently large such that \(M_\pi L \gg 1\). These two constraints \((a \sim 0.033\,\text{fm} \text{ and } M_\pi L \sim 4 - 6)\) together give the lattice size \(\sim 170^4 - 260^4\) (see Fig. 1), which is beyond the capability of the present generation of supercomputers. Nevertheless, even before the next generation of Exaflop supercomputers will be available \(\sim 2025\), one may use a smaller lattice to investigate whether the \((\mathbf{b}, \mathbf{c}, \mathbf{s})\) quarks with physical masses can be dynamically

\[
\begin{align*}
1/a &= 6\,\text{GeV}, a \sim 0.033\,\text{fm}, m_\eta a \sim 0.8 \\
M_\pi^\text{phys} \\
N_x \\
M_\pi L = 2 \\
M_\pi L = 4 \\
M_\pi L = 6 \\

\end{align*}
\]

FIG. 1: The design of lattice QCD with physical \((\mathbf{u}, \mathbf{d}, \mathbf{s}, \mathbf{c}, \mathbf{b})\) quarks.
simulated on the lattice, while keeping $u$ and $d$ quarks heavier than their physical masses. If the pion mass is kept at $\sim 700$ MeV/$c^2$, then both constraints $M_\pi L > 4$ and $m_{b,d} < 1$ can be satisfied by the $40^3 \times 64$ lattice. For domain-wall fermion with the extent $N_s = 16$ in the fifth dimension, the entire hybrid Monte Carlo (HMC) simulation \[3\] on the $40^3 \times 64 \times 16$ lattice can be performed by one GPU with at least 19 GB device memory, provided that the exact one-flavor pseudofermion action (EOFA) for domain-wall fermion \[4\] is used. In this study, we use two Nvidia GTX-TITAN-X GPU cards (each of 12 GB device memory) for each stream of HMC simulation, with the peer-to-peer communication between 2 GPUs through the PCIe bus on the motherboard.

The outline of this paper is as follows. In section 2, we recall the basics of lattice QCD with exact chiral symmetry, and discuss what is a viable framework to perform HMC simulation of lattice QCD with both heavy and light domain-wall quarks such that all topological sectors are sampled ergodically and also the chiral symmetry can be preserved to a high precision, i.e., the residual mass of any heavy/light quark flavor is negligible in comparison with its bare mass. In section 3, we describe our lattice setup. In section 4, we determine the low-lying mass spectra of mesons with valence quark contents $\bar{b}b$, $\bar{b}c$, $\bar{b}s$ and $\bar{c}c$. In section 4, we determine the masses of $(b, c, s)$ quarks. In section 5, we conclude with some remarks.

II. SIMULATION OF LATTICE QCD WITH EXACT CHIRAL SYMMETRY

A. Preliminaries

Since all quarks in QCD are excitations of Dirac fermion fields, it is vital to preserve this essential feature in lattice QCD. The most theoretically appealing lattice fermion scheme is the domain-wall/overlap fermion \[5, 7\], which preserves the exact chiral symmetry at finite lattice spacing, thus provides a proper formulation of QCD on the lattice.

To implement the exact chiral symmetry on the lattice, we use the optimal domain-wall fermion \[8\], of which the lattice fermion operator can be written as

$$[D(m_q)]_{xx'; ss'}(m_q) = (\omega_s D_w + 1)_{xx'} \delta_{ss'} + (\omega_s D_w - 1)_{xx'} L_{ss'},$$

where $\{\omega_s, s = 1, \cdots, N_s\}$ are the exact solutions such that the effective 4-dimensional lattice Dirac operator possesses the optimal chiral symmetry for any finite $N_s$. The indices $x$ and
$x'$ denote the lattice sites on the 4-dimensional lattice, and $s$ and $s'$ the indices in the fifth dimension, while the Dirac and color indices have been suppressed. Here $D_w$ is the standard Wilson Dirac operator plus a negative parameter $-m_0$ ($0 < m_0 < 2$) ($m_0$ is usually called the domain-wall height),

$$(D_w)_{xx'} = (4 - m_0) - \frac{1}{2} \sum_{\hat{\mu} = 1}^{4} \left[ (1 - \gamma_\mu)U_\mu(x)\delta_{x+\hat{\mu},x'} + (1 + \gamma_\mu)U^\dagger_\mu(x')\delta_{x-\hat{\mu},x'} \right],$$

where $U_\mu(x)$ denotes the link variable pointing from $x$ to $x+\hat{\mu}$. The operator $L$ is independent of the gauge field, and it can be written as

$$L = P_+L_+ + P_-L_-, \quad P_\pm = (1 \pm \gamma_5)/2,$$

and

$$(L_+)^{ss'} = (L_-)^{s's} = \begin{cases} -(m_q/m_{PV})\delta_{N_s,s'}, & s = 1, \\ \delta_{s-1,s'}, & 1 < s \leq N_s \end{cases},$$

where $m_q$ is the bare quark mass, and $m_{PV} = 2m_0$ is the Pauli-Villars mass for the optimal DWF. Note that the matrices $L_\pm$ satisfy $L^T_\pm = L_\mp$, and $R_5L_\pm R_5 = L_\mp$, where $R_5$ is the reflection operator in the fifth dimension, with elements $(R_5)^{ss'} = \delta_{s',N_s+1-s}$. Thus $R_5L_\pm$ is real and symmetric.

Then the pseudofermion action for the optimal DWF can be written as

$$S = \phi^\dagger \frac{D(m_{PV})}{D(m_q)} \phi, \quad m_{PV} = 2m_0,$$

where $\phi$ and $\phi^\dagger$ are complex scalar fields carrying the same quantum numbers (color, spin) of the fermion fields. Integrating the pseudofermion fields in the fermionic partition function gives the fermion determinant of the effective 4-dimensional lattice Dirac operator $D_{N_s}(m_q)$, i.e.,

$$\int [d\phi^\dagger][d\phi] \exp \left\{ -\phi^\dagger \frac{D(m_{PV})}{D(m_q)} \phi \right\} = \det \frac{D(m_q)}{D(m_{PV})} = \det D_{N_s}(m_q),$$

where

$$D_{N_s}(m_q) = m_q + \frac{1}{2}(m_{PV} - m_q)[1 + \gamma_5 S_{N_s}(H_w)],$$

$$S_{N_s}(H_w) = \frac{1 - \prod_{s=1}^{N_s} T_s}{1 + \prod_{s=1}^{N_s} T_s}, \quad T_s = \frac{1 - \omega_s H_w}{1 + \omega_s H_w}.$$
In the limit $N_s \to \infty$, $S_{N_s}(H_w) \to H_w/\sqrt{H_w^2}$, and $D_{N_s}(m_q)$ goes to
\[
D(m_q) = m_q + \frac{1}{2} (m_{PV} - m_q) \left[ 1 + \gamma_5 \frac{H_w}{\sqrt{H_w^2}} \right].
\]

In the massless limit $m_q = 0$, $D(0)$ is equal to the overlap-Dirac operator \[6\], and it satisfies the Ginsparg-Wilson relation \[9\]
\[
D(0) \gamma_5 + \gamma_5 D(0) \leftrightarrow D^{-1} \gamma_5 + \gamma_5 D^{-1} = \frac{2}{m_{PV}} \gamma_5 \mathbb{1},
\]

where the chiral symmetry is broken by a contact term, i.e., the exact chiral symmetry at finite lattice spacing. Note that (3) does not guarantee that any Ginsparg-Wilson Dirac operator $D$ must possess exact zero modes in topologically non-trivial gauge background, not to mention to satisfy the Atiyah-Singer index theorem, $Q_t = n_+ - n_-$, where $Q_t$ is the topological charge of the gauge background, and $n_\pm$ is the number of exact zero modes of $D$ with $\pm$ chirality. For example, the lattice Dirac operator constructed in Ref. \[10\] satisfies the Ginsparg-Wilson relation and possesses the correct axial anomaly in the continuum limit \[11\], but its index is always zero in any gauge background. So far, the overlap Dirac operator is the only lattice Dirac operator to possess exactly zero modes satisfying the Atiyah-Singer index theorem on a finite lattice.

However, to perform HMC simulation of lattice QCD with the overlap Dirac operator is prohibitively expensive even for a small lattice (e.g., $16^3 \times 32$), since it requires to compute the change of the number of exact zero modes $n_{\pm}$ at each step of the molecular dynamics \[12\]. Moreover, the discontinuity of the fermion determinant at the topological boundary highly suppresses the crossing rate between different topological sectors, thus renders HMC failing to sample all topological sectors ergodically. These difficulties can be circumvented by using DWF with finite $N_s$. Firstly, any positive lattice Dirac operator satisfying $\gamma_5$-hermiticity ($\gamma_5 D \gamma_5 = D^\dagger$) possesses a positive-definite pseudofermion action, without explicit dependence on $n_{\pm}$. Secondly, the step function of the fermion determinant at the topological boundary can be smoothed out by using DWF with finite $N_s$ (e.g., $N_s = 16$), then the HMC on the 5-dimensional lattice can sample all topological sectors ergodically and also keep the chiral symmetry to a high precision with the optimal DWF \[8,13\]. This has been demonstrated for $N_f = 2$ \[14\], $N_f = 1+1$ \[4\], $N_f = 2+1+1$ \[15\], and also $N_f = 2+1+1$ lattice QCD at the physical point \[16\].
B. Domain-wall fermion for heavy and light quarks

In this subsection, we discuss which variant of DWF is more capable in capturing the quantum fluctuations of both heavy and light quarks in lattice QCD.

Unlike other lattice fermions, DWF has the mass cutoff, i.e., the Pauli-Villars mass $m_{PV}$, and any quark mass has to satisfy the constraint $m_q \ll m_{PV}$. Otherwise, if $m_q \sim m_{PV}$, then $\det(m_q) / \det(m_{PV}) \sim 1$, the internal quark loops are highly suppressed, and the quantum fluctuations of the quark field become mostly quenched. In general, the Pauli-Villars mass is equal to $m_{PV} = 2m_0(1 - dm_0)$, where $d$ is a parameter depending on the variant of DWF. For the Shamir\cite{17}/Möbius\cite{18} DWF, $d = 1/2$ and $m_{PV} = m_0(2 - m_0) < 1$, since $m_0$ has to be greater than 1 ($\sim 1.3 - 1.8$) in order for its effective 4-dimensional Dirac operator to be able to detect the topology of a gauge configuration with nonzero topological charge. This imposes an upper-bound on the mass of Shamir/Möbius heavy quark on the lattice, which is more severe than the common constraint $m_q < 1$ for all lattice fermions. In other words, the Shamir/Möbius DWF is not well-suited for studying lattice QCD with heavy quarks. On the other hand, for the Borici\cite{19}/Optimal\cite{8} DWF, $d = 0$ and $m_{PV} = 2m_0 > 1$, thus provides the highest ceiling for accommodating the heavy quarks on the lattice, as well as the minimal lattice artifacts due to the mass cutoff. This can be seen by comparing the eigenvalues of their effective 4D Dirac operators in the limit $N_s \to \infty$, which is exactly equal to the overlap Dirac operator with the kernel $H = cH_w(1 + d \gamma_5 H_w)^{-1}$ in the sign function,

$$D(m_q) = m_q + \frac{1}{2}(m_{PV} - m_q) \left( 1 + \gamma_5 \frac{H}{\sqrt{H^2}} \right), \quad m_{PV} = 2m_0(1 - dm_0), \quad (4)$$

where $c = d = 1/2$ for the Shamir/Möbius DWF, while $c = 1$ and $d = 0$ for the Borici/Optimal DWF. The eigenvalues of (4) are lying on a circle in the complex plane with radius $(m_{PV} - m_q)/2$, and center at $m_q + (m_{PV} - m_q)/2$ on the real axis.

For example, fixing $m_0 = 1.3$, then $m_{PV} = 2m_0 = 2.6$ for the Borici/Optimal DWF, while $m_{PV} = m_0(2 - m_0) = 0.91$ for the Shamir/Möbius DWF. In Fig. 2 the eigenvalues of (4) are plotted for $m_q = 0$ (left panel) and $m_q = 0.8$ (right panel). Evidently, for the Shamir/Möbius DWF, the radius $(m_{PV} - m_q)/2$ of the eigenvalue circle for a heavy quark with $m_q = 0.8$ (right panel) is rather small due to $(m_{PV} - m_q)a = 0.11$, and it shrinks to zero in the limit $m_qa \to m_{PV}a = 0.91$. On the other hand, the Borici/Optimal DWF has $m_{PV}a = 2m_0 = 2.6$, and $(m_{PV} - m_q)a > 1$ for any $m_qa < 1$, thus the eigenvalues of $D(m_q)$ are not restricted to a very small circle even for the heavy quark. Moreover, in the chiral limit
C. Zolotarev optimal rational approximation and optimal domain-wall fermion

For any numerical simulation of lattice QCD with DWF, an important question is what is the optimal chiral symmetry for any finite \( N_s \) in the fifth dimension, in the sense how its effective 4D lattice Dirac operator can be exactly equal to the Zolotarev optimal rational approximation of the overlap Dirac operator. The exact solution to this problem is given in Ref. [8], with the optimal \( \{ \omega_s \} \)

\[
\omega_s = \frac{1}{\lambda_{\text{min}}} \sqrt{1 - \kappa'^2 \text{sn}^2(v_s; \kappa')}, \quad s = 1, \cdots, N_s, \tag{5}
\]

where \( \text{sn}(v_s; \kappa') \) is the Jacobian elliptic function with argument \( v_s \) (see Eq. (13) in Ref. [8]) and modulus \( \kappa' = \sqrt{1 - \lambda_{\text{min}}^2/\lambda_{\text{max}}^2} \). Then \( S_{N_s}(H_w) \) is exactly equal to the Zolotarev optimal rational approximation of \( H_w/\sqrt{H_w^2} \), i.e., the approximate sign function \( S_{N_s}(H_w) \)
satisfying the bound \(|1 - S_{N_s}(\lambda)| \leq d_Z\) for \(\lambda^2 \in [\lambda_{\text{min}}^2, \lambda_{\text{max}}^2]\), where \(d_Z\) is the maximum deviation \(|1 - \sqrt{x}R_Z(x)|_{\text{max}}\) of the Zolotarev optimal rational polynomial \(R_Z(x)\) of \(1/\sqrt{x}\) for \(x \in [1, \lambda_{\text{max}}^2/\lambda_{\text{min}}^2]\), with degree \((n - 1, n)\) for \(N_s = 2n\).

Nevertheless, the optimal weights \(\{\omega_s\}\) in [5] do not satisfy the \(R_5\) symmetry (\(\omega_s = \omega_{N_s-s+1}\)) which is required for the exact one-flavor pseudofermion action for DWF [4]. The optimal \(\{\omega_s\}\) satisfying \(R_5\) symmetry is obtained in Ref. [13]. For \(N_s = 2n\), the optimal \(\{\omega_s\}\) satisfying \(R_5\) symmetry are written as

\[
\omega_s = \omega_{N_s+1-s} = \frac{1}{\lambda_{\text{min}}} \sqrt{1 - \kappa'^2} \text{sn}^2\left(\frac{(2s - 1)K'}{N_s}; \kappa'\right), \quad s = 1, \ldots, N_s/2,
\]

where \(\text{sn}(u; \kappa')\) is the Jacobian elliptic function with modulus \(\kappa' = \sqrt{1 - \lambda_{\text{min}}^2/\lambda_{\text{max}}^2}\), and \(K'\) is the complete elliptic function of the first kind with modulus \(\kappa'\). Then the approximate sign function \(S_{N_s}(H_w)\) satisfies the bound \(0 \leq 1 - S_{N_s}(\lambda) \leq 2d_Z\) for \(\lambda^2 \in [\lambda_{\text{min}}^2, \lambda_{\text{max}}^2]\), where \(d_Z\) is defined above. Note that \(\delta(\lambda) = 1 - S(\lambda)\) does not satisfy the criterion that the maxima and minima of \(\delta(\lambda)\) all have the same magnitude but with the opposite sign (\(\delta_{\text{min}} = -\delta_{\text{max}}\)). However, the most salient features of the optimal rational approximation of degree \((m, n)\) are preserved, namely, the number of alternate maxima and minima is \((m + n + 2)\), with \((n + 1)\) maxima and \((m + 1)\) minima, and all maxima (minima) are equal to \(2d_Z\) (0). This can be regarded as the generalized optimal rational approximation (with a constant shift).

In this study, the parameters for the pseudofermion action are: \(m_0 = 1.3\), \(N_s = 2n = 16\), \(\lambda_{\text{max}}/\lambda_{\text{min}} = 6.20/0.05\), and the optimal weights \(\{\omega_s, s = 1, \ldots, N_s\}\) for the 2-flavor parts are obtained with [5], while for the one-flavor parts with [6]. In Fig. 3, the deviation of the sign function, \(\delta(\lambda) = 1 - S(\lambda)\), is plotted versus \(\lambda\), for (a) without the \(R_5\) symmetry, and (b) with the \(R_5\) symmetry. Here \(\delta(\lambda)\) has \(2n + 1 = 17\) alternate maxima and minima in the interval \([\lambda_{\text{min}}, \lambda_{\text{max}}] = [0.05, 6.2]\), with 9 maxima and 8 minima, for (a), satisfying \(-d_Z \leq 1 - S(\lambda) \leq d_Z\), while for (b), \(0 \leq 1 - S(\lambda) \leq 2d_Z\), where \(d_Z\) is the maximum deviation \(|1 - \sqrt{x}R_Z^{(7,8)}|_{\text{max}}\) of the Zolotarev optimal rational polynomial.

III. GENERATION OF THE GAUGE ENSEMBLE

In this section, we give the details of the actions, the algorithms, and the parameters to perform the HMC simulations in this study. Moreover, for the initial 257 trajectories generated by a single node (with 2 Nvidia GTX-TITAN-X GPU cards), the topological
FIG. 3: The deviation $\delta(\lambda) = 1 - S(\lambda)$ of the optimal DWF with $N_s = 2n = 16$ and $\lambda_{\text{max}}/\lambda_{\text{min}} = 6.20/0.05$, for (a) without $R_5$ symmetry, and (b) with $R_5$ symmetry.

charge fluctuation is measured, and the HMC characteristics are presented. Details of the lattice setup are given as follows.

A. The actions

In the following, we present the details of the fermion actions and the gauge action in our HMC simulations.

As noted in Ref. [15], for domain-wall fermions (DWF), to simulate $N_f = 2 + 1 + 1$ amounts to simulate $N_f = 2 + 2 + 1$. Similarly, to simulate $N_f = 2 + 1 + 1 + 1$ amounts to simulate $N_f = 2 + 2 + 1 + 1$, i.e.,

$$
\frac{(\det \mathcal{D}(m_{u/d})}{\det \mathcal{D}(m_{PV})})^2 \frac{\det \mathcal{D}(m_u)}{\det \mathcal{D}(m_{PV})} \frac{\det \mathcal{D}(m_c)}{\det \mathcal{D}(m_{PV})} \frac{\det \mathcal{D}(m_b)}{\det \mathcal{D}(m_{PV})}
$$

where only one of the 6 possible possibilities for $N_f = 2 + 2 + 1 + 1$ is written. Note that on the RHS of Eq. (7), the 2-flavor simulation with $(\det \mathcal{D}(m_c)/\det \mathcal{D}(m_{PV}))^2$ is more efficient than its counterpart of one-flavor with $(\det \mathcal{D}(m_c)/\det \mathcal{D}(m_{PV}))$ on the LHS. Moreover, the one-flavor simulation with $\det \mathcal{D}(m_s)/\det \mathcal{D}(m_c)$ on the RHS is more efficient than the original
one with \( \det \mathcal{D}(m_a) / \det \mathcal{D}(m_{PV}) \) on the LHS. Thus, we perform the HMC simulation with
the expression on the RHS of Eq. (7).

For the two-flavor parts, \((\det \mathcal{D}(m_{u/d}) / \det \mathcal{D}(m_{PV}))^2 \) and \((\det \mathcal{D}(m_c) / \det \mathcal{D}(m_{PV}))^2 \), we use the \( N_f = 2 \) pseudofermion action which has been using since 2011 [14], and it can be
written as

\[
S(m_q, m_{PV}) = \phi \dagger C \dagger (m_{PV}) \{C(m_q)C \dagger (m_q)\}^{-1}C(m_{PV})\phi, \quad m_{PV} = 2m_0, \tag{8}
\]

where

\[
C(m_q) = 1 - M_5(m_q)D_w^{OE}M_5(m_q)D_w^{EO},
\]

\[
M_5(m_q) = \{4 - m_0 + \omega^{-1/2}[1 - L(m_q)][(1 + L(m_q))^{-1}\omega^{-1/2}]^{-1},
\]

and \( L(m_q) \) is defined in [1] and [2]. Here \( \omega \equiv \text{diag}\{\omega_1, \omega_2, \cdots, \omega_{N_5}\} \) is a diagonal matrix
in the fifth dimension, and \( D_w^{EO/OE} \) denotes the part of \( D_w \) with gauge links pointing from
even/odd sites to odd/even sites after even-odd preconditioning on the 4-dimensional lattice.

For the two-flavor part of \( u \) and \( d \) quarks, we turn on the mass-preconditioning \([20]\)
by introducing an auxiliary heavy fermion field with mass \( m_Ha = 0.1 \). Then the \( N_f = 2 \)
pseudofermion action \([8]\) is replaced with

\[
S(m_q, m_H) + S(m_H, m_{PV}) = \phi \dagger C(m_H) \dagger \{C(m_q)C(m_q)\}^{-1}C(m_H)\phi + \phi_H \dagger C \dagger (m_{PV}) \{C(m_H)C(m_H)\}^{-1}C(m_{PV})\phi_H,
\]

which gives the partition function (fermion determinant) exactly the same as that of (8).

For the one-flavor parts, \( \det \mathcal{D}(m_a) / \det \mathcal{D}(m_c) \) and \( \det \mathcal{D}(m_b) / \det \mathcal{D}(m_{PV}) \), we use the
exact one-flavor pseudofermion action (EOFA) for DWF \([4]\). For the optimal DWF, it can
be written as \( (m_1 < m_2) \)

\[
\frac{\det \mathcal{D}(m_1)}{\det \mathcal{D}(m_2)} = \frac{\det \mathcal{T}(m_1)}{\det \mathcal{T}(m_2)} = \int d\phi_+^\dagger d\phi_- \exp \left(-\phi_+^\dagger G_+(m_1, m_2)\phi_+ - \phi_+^\dagger G_-(m_1, m_2)\phi_-\right), \tag{9}
\]

where \( \phi_\pm \) and \( \phi_\pm^\dagger \) are pseudofermion fields (each of two spinor components) on the 4-dimensional lattice, and

\[
G_-(m_1, m_2) = P_- \left[I - k(m_1, m_2)\omega^{-1/2}v_-^Tv_-^T\frac{1}{H_T(m_1)}v_\omega^{-1/2}\right] P_-,
\]

\[
G_+(m_1, m_2) = P_+ \left[I + k(m_1, m_2)\omega^{-1/2}v_+^Tv_+^T\frac{1}{H_T(m_2)} - \Delta_+(m_1, m_2)P_+ v_+^Tv_\omega^{-1/2}\right] P_+. \tag{10}
\]
Here

\[ D_T(m_i) = D_w + M(m_i), \quad i = 1, 2 \]

\[ M(m_i) = \omega^{-1/2}[1 - L(m_i)][1 + L(m_i)]^{-1} \omega^{-1/2} = P_+ M_+(m_i) + P_- M_-(m_i), \]

\[ H_T(m_i) = R_5 \gamma_5 D_T(m_i), \]

\[ \Delta(m_1, m_2) = R_5 [M(m_2) - M(m_1)] = P_+ \Delta_+(m_1, m_2) + P_- \Delta_-(m_1, m_1), \]

\[ \Delta_\pm(m_1, m_2) = k(m_1, m_2) \omega^{-1/2} v_\pm v_\mp^T \omega^{-1/2}, \]

\[ k(m_1, m_2) = \frac{m_2 - m_1}{m_2 + m_1}, \]

\[ v_\mp^T = (-1, 1, \cdots, (-1)^N), \quad v_- = -v_+. \]

For the gluon fields, we use the Wilson plaquette gauge action at \( \beta = 6/g_0^2 = 6.70. \)

\[ S_g(U) = \frac{6}{g_0^2} \sum_{\text{plaq.}} \left\{ 1 - \frac{1}{3} \text{ReTr}(U_p) \right\}, \]

where \( g_0 \) is the bare coupling.

The bare mass of \( u/d \) quarks is set to \( m_u/d = 0.01 \) such that \( M_\pi L > 4 \), while the bare masses of \( (b, c, s) \) are tuned to \( (m_b, m_c, m_s) = (0.85, 0.20, 0.15) \) such that they give the masses of the vector mesons \( \Upsilon(9460), J/\psi(3097) \), and \( \phi(1020) \) respectively. The algorithm for simulating 2-flavor action for optimal domain-wall quarks has been outlined in Ref. [14], while that for simulating the exact one-flavor pseudofermion action (EOFA) of domain-wall fermion has been presented in Refs. [4, 21]. In the molecular dynamics, we use the Omelyan integrator [23], the multiple-time scale method [24], and the mass-preconditioning [20].

**B. HMC simulations**

Following the common strategy to reduce the thermalization time for a large lattice such as \( 40^3 \times 64 \), we first perform the thermalization on a smaller lattice \( 20^3 \times 32 \) with the same set of parameters \( (\beta, m_u/d, m_s, m_c, m_b) \). Then the thermalized gauge configuration on the \( 20^3 \times 32 \) lattice is used to construct the initial gauge configuration on the \( 40^3 \times 64 \) lattice by doubling the size of the lattice in each direction with the periodic extension. With this initial gauge configuration, we generate the first 257 trajectories on the \( 40^3 \times 64 \) lattice with two Nvidia GTX-TITAN-X GPU cards, each with device memory 12 GB. After discarding the initial 187 trajectories for thermalization, we sample one configuration every 5
FIG. 4: The maximum forces of the gauge field, the 2-flavor pseudofermion fields, and the one-flavor pseudofermion fields versus the HMC trajectory in the HMC simulations of the lattice QCD with $N_f = 2 + 1 + 1 + 1$ optimal DWF.

trajectories, resulting 14 “seed” configurations. Then we use these seed configurations as the initial configurations for 14 independent simulations on 14 nodes, each of two Nvidia GTX-TITAN-X GPU cards. Each node generates $\sim 40$ trajectories independently, and all 14 nodes accumulate a total of 535 trajectories. We sample one configuration every 5 trajectories in each stream, and obtain a total of 103 configurations for physical measurements.

In the following, we summarize the HMC characteristics of the first 257 trajectories. In Fig. 4 we plot the maximum force (averaged over all links) among all momentum updates in each trajectory, for the gauge force, the 2-flavor pseudofermion forces, and the one-flavor pseudofermion forces respectively, where $\phi(m_1/m_2)$ denotes the two-flavor fermion force due to the pseudofermion action $S(m_1, m_2)$, and $\phi_\pm(m_1/m_2)$ denotes the one-flavor pseudofermion force due to the exact one-flavor action with $\pm$ chirality, $S_\pm(m_1, m_2) =$
FIG. 5: The change of the Hamiltonian $\Delta H$ versus the trajectory in the HMC simulations of lattice QCD with $N_f = 2+1+1+1$ optimal DWF. The line connecting the data points is only for guiding the eyes.

$\phi_+^\dagger G_\pm (m_1, m_2) \phi_\pm$. From the sizes of various forces in Fig. 4, the multiple time scales can be designed in the momentum update with the gauge force and the pseudofermion forces. With the length of the HMC trajectory equal to one, we use 4 different time scales for the momentum updates with (1) the gauge force; (2) the two-flavor fermion forces associated with $\phi(m_c/m_{PV})$ and $\phi(m_H/m_{PV})$; (3) the two-flavor force associated with $\phi(m_u/m_H)$ and the one-flavor fermion force associated with $\phi_+(m_b/m_{PV})$; (4) the one-flavor fermion forces associated with $\phi_-(m_b/m_{PV})$, $\phi_+(m_s/m_c)$, and $\phi_-(m_s/m_c)$, which correspond to the step sizes $1/(k_1k_2k_3k_4)$, $1/(k_2k_3k_4)$, $1/(k_3k_4)$, and $1/k_4$ respectively. In our simulation, we set $(k_1, k_2, k_3, k_4) = (10, 2, 2, 5)$.

In Fig. 5, the change of Hamiltonian $\Delta H$ versus the HMC trajectory is plotted for the first 257 trajectories, with $\langle \Delta H \rangle = 0.376(57)$. The number of accepted trajectories is 173, giving the acceptance rate 0.673(29). Using the measured value of $\langle \Delta H \rangle = 0.376(57)$, we can obtain the theoretical estimate of the acceptance rate with the formula $P_{\text{acc}} = \text{erfc} \left( \frac{\sqrt{\langle \Delta H \rangle}}{2} \right)$ \cite{25}, which gives 0.664(24), in good agreement with the measured acceptance rate 0.673(29). Moreover, we measure the expectation value of $\exp(-\Delta H)$, to check whether it is consistent with the theoretical formula $\langle \exp(-\Delta H) \rangle = 1$ which follows from the area-preserving property of the HMC simulation \cite{26}. The measured value of $\langle \exp(-\Delta H) \rangle$ is 1.026(66), in good
agreement with the theoretical expectation value. The summary of the HMC characteristics for the initial 257 trajectories is given in Table I.

**TABLE I:** Summary of the HMC characteristics for the first 257 trajectories in the simulation of \(N_f = 2 + 1 + 1 + 1\) lattice QCD with the optimal DWF.

| \(N_{\text{traj}}\) | Time(s)/traj | Acceptance | \(\langle \Delta H \rangle\) | \(P_{\text{acc}} = \text{erfc}(\sqrt{\langle \Delta H \rangle}/2)\) | \(\langle \exp(-\Delta H) \rangle \langle \text{plaquette} \rangle\) |
|-------------------|--------------|------------|------------------|--------------------------------|--------------------------------|
| 257               | 76349(146)   | 0.673(29)  | 0.376(57)        | 0.664(24)                      | 1.026(66)                      |

C. **Topological charge fluctuations**

In this subsection, we examine the evolution of the topological charge \(Q_t\) in the first 257 trajectories, and obtain the histogram of its distribution.

In lattice QCD with exact chiral symmetry, the topological charge \(Q_t\) can be measured by the index of the massless overlap-Dirac operator, since its index satisfies the Atiyah-Singer index theorem, \(\text{index}(D_{\text{ov}}) = n_+ - n_- = Q_t\). However, to project the zero modes of the massless overlap-Dirac operator for the \(40^3 \times 64\) lattice is prohibitively expensive. On the other hand, the clover topological charge \(Q_{\text{clover}} = \sum_x \epsilon_{\mu\nu\lambda\sigma} \text{tr}[F_{\mu\nu}(x)F_{\lambda\sigma}(x)]/(32\pi^2)\) is not reliable [where the matrix-valued field tensor \(F_{\mu\nu}(x)\) is obtained from the four plaquettes surrounding \(x\) on the \((\hat{\mu}, \hat{\nu})\) plane], unless the gauge configuration is sufficiently smooth. Nevertheless, the smoothness of a gauge configuration can be attained by the Wilson flow \([27, 28]\), which is a continuous-smearing process to average gauge field over a spherical region of root-mean-square radius \(R_{\text{rms}} = \sqrt{8t}\), where \(t\) is the flow-time. In this study, the flow equation is numerically integrated from \(t = 0\) with \(\Delta t/a^2 = 0.01\), and measure the \(Q_{\text{clover}}\) at \(t/a^2 = 0.4\) which amounts to averaging the gauge field over a spherical region of root-mean-square radius \(R_{\text{rms}} = \sqrt{8t} \sim 1.8a\). Then each gauge configuration becomes very smooth, with \(Q_{\text{clover}}\) close to an integer, and the average plaquette greater than 0.997. Denoting the nearest integer of \(Q_{\text{clover}}\) by \(Q_t \equiv \text{round}(Q_{\text{clover}})\), \(Q_t\) is plotted versus the trajectory number in the left-panel of Fig. 6, while the right-panel displays the histogram of the probability distribution of \(Q_t\) of the first 257 HMC trajectories. Evidently, the HMC simulation samples all topological sectors ergodically. Note that the lattice volume is rather
small, $\sim (1.2 \text{ fm})^3 \times (1.9 \text{ fm})$, thus the chance of sampling $Q_t > 3$ is literally zero for 257 trajectories.

![Graph of $Q_t$ versus trajectory](image)

**FIG. 6**: (left panel) The evolution of $Q_t$ versus the HMC trajectory. The line connecting the data points is only for guiding the eyes. (right panel) The histogram of the probability distribution of $Q_t$ for the first 257 HMC trajectories.

### D. Lattice scale

First, we recap the generation of the gauge ensemble. From the initial 257 trajectories generated by a single node, we discard the first 187 trajectories for thermalization, and sample one configuration every 5 trajectories, resulting 14 “seed” configurations. Then we use these seed configurations as the initial configurations for 14 independent simulations on 14 nodes, each of two Nvidia GTX-TITAN-X GPU cards. Each node generates $\sim 40$ trajectories independently, and all 14 nodes accumulate a total of 535 trajectories. We sample one configuration every 5 trajectories in each stream, and obtain a total of 103 configurations for physical measurements.

To determine the lattice scale, we use the Wilson flow [27, 28] with the condition

$$\{t^2 \langle E(t) \rangle \}_{t=t_0} = 0.3,$$

and obtain $\sqrt{t_0}/a = 4.6884(36)$ for the 103 configurations for physical measurements. Using $\sqrt{t_0} = 0.1416(8) \text{ fm}$ obtained by the MILC Collaboration for the $(2 + 1 + 1)$-flavors QCD
we have $a^{-1} = 6.503 \pm 0.037$ GeV. The lattice spacing is $a = 0.0303(2)$ fm, giving the spatial volume $\sim (1.213 \text{ fm})^3$, which is too small for studying physical observables involving the light quarks.

**E. Quark propagator**

We compute the valence quark propagator of the effective 4D Dirac operator with the point source at the origin, and with the mass and other parameters exactly the same as those of the sea quarks. The boundary conditions are periodic in space and antiperiodic in time. First, we solve the following linear system with mixed-precision conjugate gradient algorithm, for the even-odd preconditioned $D$

$$D(m_q)|Y\rangle = D(m_{PV})B^{-1}|\text{source vector}\rangle,$$

where $B_{x,s,x',s'}^{-1} = \delta_{x,x'}(P_-\delta_{s,s'} + P_+\delta_{s+1,s'})$ with periodic boundary conditions in the fifth dimension. Then the solution of (12) gives the valence quark propagator

$$(D_c + m_q)^{-1}_{x,x'} = (m_{PV} - m_q)^{-1}[(BY)_{x,1;x',1} - \delta_{x,x'}], \quad m_{PV} = 2m_0.$$  

(13)

Each column of the quark propagator is computed by a single node with 2 Nvidia GTX-TITAN-X GPU cards, which attains more than 1000 Gflops/sec (sustained).

**F. Residual masses**

To measure the chiral symmetry breaking due to finite $N_s$, we compute the residual mass according to [31],

$$m_{\text{res}} = \left\langle \frac{\text{tr}(D_c + m_q)^{-1}_{0,0}}{\text{tr}[\gamma_5(D_c + m_q)\gamma_5(D_c + m_q)]^{-1}_{0,0}} \right\rangle - m_q,$$

where $(D_c + m_q)^{-1}$ denotes the valence quark propagator with $m_q$ equal to the sea-quark mass, tr denotes the trace running over the color and Dirac indices, and the brackets $\langle \cdots \rangle$ denote the averaging over the gauge ensemble. In the limit $N_s \to \infty$, $D_c$ is exactly chiral symmetric and the first term on the RHS of (14) is exactly equal to $m_q$, thus the residual mass $m_{\text{res}}$ is exactly zero, and the quark mass $m_q$ is well-defined for each gauge configuration. On the other hand, for any finite $N_s$ with nonzero residual mass, the quark mass is not
well-defined for each gauge configuration, but its impact on any physical observable can be roughly estimated by the difference due to changing the valence quark mass from \( m_q \) to \( m_q + m_{\text{res}} \).

**TABLE II: The residual masses of \( u/d, s, c, \) and \( b \) quarks.**

| quark   | \( m_q a \)  | \( m_{\text{res}} a \)     | \( m_{\text{res}} \) [MeV] |
|---------|--------------|------------------------------|-----------------------------|
| u/d     | 0.010        | 7.93(52) \( \times 10^{-7} \) | 0.0052(3)                   |
| s       | 0.015        | 8.21(52) \( \times 10^{-7} \) | 0.0053(3)                   |
| c       | 0.200        | 9.43(54) \( \times 10^{-7} \) | 0.0061(4)                   |
| b       | 0.850        | 1.06(60) \( \times 10^{-6} \) | 0.0069(4)                   |

For the 103 gauge configurations generated by HMC simulation of lattice QCD with \( N_f = 2 + 1 + 1 + 1 \) optimal domain-wall quarks, the residual masses of \( u/d, s, c, \) and \( b \) quarks are listed in Table II. We see that the residual mass of any quark flavor is less than 0.007 MeV, which should be negligible in comparison with other systematic uncertainties.

**IV. MASS SPECTRA OF BEAUTY MESONS**

In the following, we determine the masses of the low-lying mesons with valence quark contents \( \bar{b}b, \bar{b}c, \bar{b}s, \) and \( \bar{c}c \). We construct the quark-antiquark meson interpolators and measure their time-correlation functions using the point-to-point quark propagators computed with the same parameters \( (N_s = 16, m_0 = 1.3, \lambda_{\text{max}}/\lambda_{\text{min}} = 6.20/0.05) \) of the sea quarks, for the quark masses \( (m_{u/d} a = 0.01, m_s a = 0.015, m_c a = 0.20, m_b a = 0.85) \), where \( m_b, m_c \) and \( m_s \) are fixed by the masses of the vector mesons \( \Upsilon(9460), J/\psi(3097), \) and \( \phi(1020) \) respectively. Then we extract the mass of the lowest-lying meson state from the time-correlation function.

The time-correlation function of the beauty meson interpolator \( \bar{b}\Gamma q \) (where \( q = \{b, c, s\} \)) is measured according to the formula

\[
C_{\Gamma}(t) = \left\langle \sum_{\vec{x}} \text{tr}\{\Gamma(D_c + m_b)_{x,0}^{-1}\Gamma(D_c + m_q)_{0,x}^{-1}\} \right\rangle, \tag{15}
\]

where \( \Gamma = \{1, \gamma_5, \gamma_i, \gamma_5 \gamma_i, \epsilon_{ijk} \gamma_j \gamma_k\} \), corresponding to scalar \( (S) \), pseudoscalar \( (P) \), vector \( (V) \), axial-vector \( (A) \), and pseudovector \( (T) \) respectively, and the valence quark propagator
$(D_c + m_q)^{-1}$ is computed according to the formula [13]. Note that $\bar{q}\gamma_5\gamma_iq$ transforms like $J^{PC} = 1^{++}$, while $\bar{q}\epsilon_{ijk}\gamma_j\gamma_kq$ like $J^{PC} = 1^{+-}$.

For the vector meson, we average over $i = 1, 2, 3$ components, namely,

$$C_V(t) = \left\langle \frac{1}{3} \sum_{i=1}^{3} \sum_x \text{tr}\{\gamma_i(D_c + m_b)_{x,0}^{-1} \gamma_i(D_c + m_q)_{0,x}^{-1}\} \right\rangle.$$

Similarly, we perform the same averaging for the axial-vector and pseudovector mesons. Moreover, to enhance statistics, we average the forward and the backward time-correlation function.

$$\bar{C}(t) = \frac{1}{2} [C(t) + C(T - t)].$$

The time-correlation function (TCF) and the effective mass of the meson interpolators $\bar{b}\Gamma b$, $\bar{c}\Gamma c$, $\bar{b}\Gamma c$, and $\bar{s}\Gamma s$ are plotted in the Appendices A-D respectively.

### A. Bottomonium and Charmonium

First of all, we check to what extent we can reproduce the bottomonium masses which have been measured precisely in high energy experiments.

Our results of the mass spectrum of the low-lying states of bottomonium are summarized in Table III. The time-correlation function and the effective mass of $\bar{b}\Gamma b$ are plotted in Appendix A.

The first column in Table III is the Dirac matrix used for computing the time-correlation function (15). The second column is $J^{PC}$ of the state. The third column is the $[t_1, t_2]$ used for fitting the data of $C_F(t)$ to the usual formula

$$\frac{z^2}{2Ma} [e^{-Ma t} + e^{-Ma(T-t)}]$$

(16) to extract the ground state meson mass $M$, where the excited states have been neglected. We use the correlated fit throughout this work. The fifth column is the mass $M$ of the meson state, where the first error is statistical, and the second is systematic. Here the statistical error is estimated using the jackknife method with the bin size of which the statistical error saturates, while the systematic error is estimated based on all fittings satisfying $\chi^2/\text{dof} < 1.2$ and $|t_2 - t_1| \geq 6$ with $t_1 \geq 10$ and $t_2 \leq 32$. The last column is the experimental state we have identified, and its PDG mass value [32].
The analysis and the descriptions in the above paragraph apply to all results obtained in this work, as given in Table [III][VI].

TABLE III: The masses of low-lying bottomonium states obtained in this work. The fifth column is the mass of the meson state, where the first error is statistical, and the second is systematic. The last column is the experimental state we have identified, and its PDG mass value [32]. For a detailed description of each column, see the paragraph with Eq. [16].

| Γ     | $J^{PC}$ | $[t_1, t_2]$ | $\chi^2$/dof | Mass(MeV)   | PDG  |
|-------|---------|-------------|--------------|-------------|-----|
| I     | 0$^{++}$| [19,29]     | 1.10         | 9859(14)(11) | $\chi_b(9859)$ |
| $\gamma_5$ | 0$^{-+}$| [15,31]     | 1.04         | 9403(4)(5)  | $\eta_b(9399)$ |
| $\gamma_i$ | 1$^{--}$| [21,31]     | 0.51         | 9468(7)(6)  | $\Upsilon(9460)$ |
| $\gamma_5\gamma_i$ | 1$^{++}$| [19,26]     | 1.15         | 9884(27)(35)| $\chi_b\prime(9893)$ |
| $\epsilon_{ijk}\gamma_j\gamma_k$ | 1$^{+-}$| [19,25]     | 0.97         | 9910(20)(25)| $h_b(9899)$ |

Evidently, the masses of bottomonium in Table [III] are in good agreement with the PDG mass values, even though the axial-vector (1$^{--}$) and pseudovector (1$^{+-}$) mesons have relatively larger errors than other meson states.

TABLE IV: The masses of low-lying charmonium states obtained in this work. The fifth column is the mass of the meson state, where the first error is statistical, and the second is systematic. The last column is the experimental state we have identified, and its PDG mass value [32]. For a detailed description of each column, see the paragraph with Eq. [16].

| Γ     | $J^{PC}$ | $[t_1, t_2]$ | $\chi^2$/dof | Mass(MeV)   | PDG  |
|-------|---------|-------------|--------------|-------------|-----|
| I     | 0$^{++}$| [14,25]     | 1.01         | 3403(16)(13)| $\chi_c(3415)$ |
| $\gamma_5$ | 0$^{-+}$| [15,29]     | 1.17         | 2989(6)(4)  | $\eta_c(2984)$ |
| $\gamma_i$ | 1$^{--}$| [15,28]     | 0.65         | 3112(7)(5)  | $J/\psi(3097)$ |
| $\gamma_5\gamma_i$ | 1$^{++}$| [14,21]     | 1.13         | 3513(23)(10)| $\chi_c\prime(3510)$ |
| $\epsilon_{ijk}\gamma_j\gamma_k$ | 1$^{+-}$| [17,25]     | 0.39         | 3527(14)(19)| $h_c(3524)$ |

Next, we turn to the charmonium states extracted from the ground states of $\bar{c}\Gamma c$. Our
results of the masses of the low-lying states of charmonium are summarized in Table IV. The time-correlation function and the effective mass of $\bar{c}\Gamma c$ are plotted in Appendix B. Evidently, the theoretical masses of charmonium in Table IV are in good agreement with the PDG values. Note that the theoretical result of the hyperfine splitting ($1^3S_1 - 1^1S_0$) is $123(9)(6) \text{ MeV}$, in good agreement with the PDG value $118 \text{ MeV}$.

B. $B_s$ and $B_c$ mesons

Our results of the masses of the low-lying states of $B_s$ mesons are summarized in Table V. The time-correlation function and the effective mass of $\bar{b}\Gamma s$ are plotted in Appendix D. Here we have identified the scalar $\bar{b}s$ meson with the state $B_{sJ}^*(5850)$ observed in high energy experiments, due to the proximity of their masses. This predicts that $B_{sJ}^*(5850)$ possesses $J^P = 0^+$, which can be verified by high energy experiments in the future. Moreover, the pseudovector meson (the last entry in Table V) has not been observed in high energy experiments, thus it serves as a prediction of $N_f = 2 + 1 + 1 + 1$ lattice QCD.

TABLE V: The masses of low-lying $B_s$ meson states obtained in this work. The fifth column is the mass of the meson state, where the first error is statistical, and the second is systematic. The last column is the experimental state we have identified, and its PDG mass value \[32\]. For a detailed description of each column, see the paragraph with Eq. (16).

| $\Gamma$   | $J^P$ | $[t_1,t_2]$ | $\chi^2$/dof | Mass(MeV)   | PDG            |
|------------|-------|-------------|--------------|-------------|----------------|
| $1$        | $0^+$ | [15,24]     | 0.37         | 5839(30)(18) | $B_{sJ}^*(5850)$ |
| $\gamma_5$| $0^-$ | [23,29]     | 0.79         | 5406(16)(17) | $B_s(5367)$     |
| $\gamma_i$| $1^-$ | [18,29]     | 0.66         | 5430(17)(18) | $B_s^*(5415)$   |
| $\gamma_5\gamma_i$| $1^+$ | [16,22]     | 0.58         | 5839(23)(14) | $B_{s1}(5830)$  |
| $\epsilon_{ijk}\gamma_j\gamma_k$| $1^+$ | [16,23]     | 0.56         | 5909(26)(34) |                |

Finally, we turn to the heavy mesons with beauty and charm. In Table VI, we summarize our results of the masses of $B_c$ mesons extracted from the ground states of $\bar{b}\Gamma c$. The time-correlation function and the effective mass of $\bar{b}\Gamma c$ are plotted in the Appendix C. Except for the pseudoscalar meson $B_c(6275)$, other four meson states have not been observed in
high energy experiments. It is interesting to see to what extent the experimental results will agree with our theoretical predictions.

TABLE VI: The masses of low-lying $B_c$ meson states obtained in this work. The fifth column is the mass of the meson state, where the first error is statistical, and the second is systematic. The last column is the experimental state we have identified, and its PDG mass value [32]. For a detailed description of each column, see the paragraph with Eq. (16).

| $\Gamma$  | $J^P$ | $[t_1,t_2]$ | $\chi^2$/dof | Mass(MeV)      | PDG         |
|----------|-------|-------------|--------------|----------------|-------------|
| I        | $0^+$ | $[20,28]$   | 1.17         | 6766(38)(16)   |             |
| $\gamma_5$ | $0^-$ | $[15,31]$   | 1.02         | 6285(6)(5)     | $B_c(6275)$|
| $\gamma_i$ | 1$^-$ | $[16,31]$   | 0.68         | 6375(6)(7)     |             |
| $\gamma_5\gamma_i$ | 1$^+$ | $[21,32]$   | 0.62         | 6787(34)(28)   |             |
| $\epsilon_{ijk}\gamma_j\gamma_k$ | 1$^+$ | $[19,26]$   | 0.97         | 6798(33)(17)   |             |

V. QUARK MASSES OF (b, c, s)

The quark masses cannot be measured directly in high energy experiments since quarks are confined inside hadrons. Therefore, the quark masses can only be determined by comparing theoretical calculations of physical observables with the experimental values. For any field theoretic calculation, the quark masses depend on the regularization, as well as the renormalization scheme and scale. For lattice QCD, the hadron masses can be computed nonperturbatively from the first principles, and from which the quark masses can be determined.

We have used the mass of the vector meson $\Upsilon(9460)$ to fix the bare mass of $b$ quark equal to $m_b = 0.850(5)a^{-1}$. To transcribe the bare mass to the corresponding value in the usual renormalization scheme $\overline{\text{MS}}$ in high energy phenomenology, one needs to compute the lattice renormalization constant $Z_m = Z_s^{-1}$, where $Z_s$ is the renormalization constant for $\bar{\psi}\psi$. In general, $Z_m$ should be determined nonperturbatively. However, in this study, the lattice spacing is rather small ($a \simeq 0.03$ fm), thus it is justified to use the one-loop perturbation
formula [33]

\[ Z_s(\mu) = 1 + \frac{g^2}{4\pi^2} \left[ \ln(a^2\mu^2) + 0.17154 \right] \quad (m_0 = 1.30). \]  

(17)

At \( \beta = 6.70, \ a^{-1} = 6.503(37) \) GeV, and \( \mu = 2 \) GeV, \( Z_s = 1.1001(2) \), which transcribes the bare mass \( m_b \) to the \( \overline{\text{MS}} \) mass at \( \mu = 2 \) GeV

\[ \overline{m}_b(2 \text{ GeV}) = m_b Z_m(2 \text{ GeV}) = 5.024 \pm 0.025 \text{ GeV}, \]

where the error bar combines (in quadrature) the statistical error and the systematic errors of the lattice spacing and the b quark bare mass.

To compare our result with the PDG value of \( m_b(\overline{m}_b) \) at the scale \( \mu = \overline{m}_b \), we solve the equation \( \overline{m}_b = m_b Z_m(\mu = \overline{m}_b) \) and obtain

\[ \overline{m}_b(\overline{m}_b) = 4.85 \pm 0.04 \text{ GeV}, \]

(18)

which is higher than the PDG value \( (4.18 \pm 0.03) \text{ GeV} \) for \( N_f = 2 + 1 + 1 \) lattice QCD, but is closer to the value in the 1S scheme \( m_b^{1S} = 4.65(3) \text{ GeV} \) [32].

Next we turn to the charm quark mass. Using (17), the charm quark bare mass \( m_c = 0.200(5)a^{-1} \) is transcribed to

\[ \overline{m}_c(2 \text{ GeV}) = 1.14 \pm 0.03 \text{ GeV}, \]

where the error bar combines (in quadrature) the statistical and the systematic errors from the lattice spacing and the charm quark bare mass. To compare our result with the PDG value of \( m_c(\overline{m}_c) \), we solve \( \overline{m}_c = m_c Z_m(\mu = \overline{m}_c) \) and obtain

\[ \overline{m}_c(\overline{m}_c) = 1.21 \pm 0.03 \text{ GeV}, \]

(19)

which is slightly smaller than the PDG value \( (1.280 \pm 0.025) \text{ GeV} \) for \( N_f = 2 + 1 + 1 \) lattice QCD [32].

Finally we turn to the strange quark mass. Using (17), the strange quark bare mass \( m_s = 0.0150(2)a^{-1} \) is transcribed to

\[ \overline{m}_s(2 \text{ GeV}) = 88.7 \pm 1.3 \text{ MeV}, \]

(20)

where the error bar combines (in quadrature) the statistical and the systematic ones from the lattice spacing and the s quark bare mass. Our result of the strange quark mass (20) is slightly smaller than the PDG value \( (92.9 \pm 0.7) \text{ MeV} \) for \( N_f = 2 + 1 + 1 \) lattice QCD [32].
VI. CONCLUDING REMARK

This study demonstrates that the Dirac b quark can be simulated dynamically in lattice QCD, together with the (c, s, d, u) quarks. Even with unphysically heavy u and d quarks in the sea, the low-lying mass spectra of mesons with valence quark contents $\bar{b}b$, $\bar{b}c$, $\bar{b}s$, and $\bar{c}c$ are in good agreement with the experimental values. Also, we have several predictions which have not been observed in high energy experiments, i.e., predicting the mass and the $J^P$ of four $B_c$ meson states (see Table VI), the $J^P$ of $B_{sJ}^*(5850)$ to be $0^+$, and the mass and the $J^P$ of the pseudovector $B_s$ meson state (see Table V). Moreover, we have determined the masses of (b, c, s) quarks, as given in (18), (19), and (20) respectively.

These results imply that it is feasible to simulate lattice QCD with physical (u, d, s, c, b) domain-wall quarks on a large ($\sim 200^4$) lattice, with the Exaflops supercomputers which will be available $\sim 2025$. Then physical observables with any (u, d, s, c, b) quark contents can be computed from the first principles of QCD. This will provide a viable way to systematically reduce the uncertainties in the theoretical predictions of the Standard Model (SM), which are largely stemming from the sector of the strong interaction\cite{34}. This is crucial for unveiling any new physics beyond the standard model (SM), by identifying any discrepancies between the high energy experimental results and the theoretical values derived from the first principles of the SM with all quarks (heavy and light) as Dirac fermions, without using non-relativistic approximation or heavy quark effective field theory for b and c quarks.

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Appendix A: $C(t)$ and the effective mass of $\bar{b}\gamma_5 b$

FIG. 7: The time-correlation function and the effective mass of the meson interpolator $\bar{b}\gamma_5 b$.

FIG. 8: The time-correlation function and the effective mass of the meson interpolator $\bar{b}\gamma_i b$. 
FIG. 9: The time-correlation function and the effective mass of the meson interpolator $\bar{b}b$.

FIG. 10: The time-correlation function and the effective mass of the meson interpolator $\bar{b}\gamma_5\gamma_i b$. 
FIG. 11: The time-correlation function and the effective mass of the meson interpolator $\bar{b}\epsilon_{ijk}\gamma_j\gamma_k b$. 
Appendix B: $C(t)$ and the effective mass of $\bar{c}\gamma^c$

**FIG. 12:** The time-correlation function and the effective mass of the meson interpolator $\bar{c}\gamma^5c$.

**FIG. 13:** The time-correlation function and the effective mass of the meson interpolator $\bar{c}\gamma^i c$. 

$\Gamma = \gamma^5$ (pseudoscalar) 

$\Gamma = \gamma_i$ (vector)
FIG. 14: The time-correlation function and the effective mass of the meson interpolator $\bar{c}c$.

FIG. 15: The time-correlation function and the effective mass of the meson interpolator $\bar{c}\gamma_5\gamma_ic$. 
FIG. 16: The time-correlation function and the effective mass of the meson interpolator $\bar{c}\epsilon_{ijk}\gamma_j\gamma_k c$. 
Appendix C: $C(t)$ and the effective mass of $\bar{b}\Gamma c$

FIG. 17: The time-correlation function and the effective mass of the meson interpolator $\bar{b}\gamma_5 c$.

FIG. 18: The time-correlation function and the effective mass of the meson interpolator $\bar{b}\gamma_i c$. 
FIG. 19: The time-correlation function and the effective mass of the meson interpolator $\bar{b}c$.

FIG. 20: The time-correlation function and the effective mass of the meson interpolator $\bar{b}\gamma_5\gamma_\gamma c$. 
FIG. 21: The time-correlation function and the effective mass of the meson interpolator \( \bar{b} \epsilon_{ijk} \gamma_j \gamma_k c \).
Appendix D: $C(t)$ and the effective mass of $\bar{b}\gamma_5$s

**FIG. 22:** The time-correlation function and the effective mass of the meson interpolator $\bar{b}\gamma_5$s.

**FIG. 23:** The time-correlation function and the effective mass of the meson interpolator $\bar{b}\gamma_i$s.
FIG. 24: The time-correlation function and the effective mass of the meson interpolator $\bar{b}s$.

FIG. 25: The time-correlation function and the effective mass of the meson interpolator $\bar{b}\gamma_5 \gamma_i s$. 

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FIG. 26: The time-correlation function and the effective mass of the meson interpolator $\bar{b}\epsilon^{ijk}\gamma^i\gamma^j\gamma^k$. 