# A new method to access heavy meson lightcone distribution amplitudes from first-principle

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We present a method to compute lightcone distribution amplitudes (LCDAs) of heavy meson within heavy quark effective theory (HQET). Our method utilizes quasi distribution amplitudes (quasi-DAs) with a large momentum component $P^z$. We point out that by sequentially integrating out $P^z$ and $m_H$, one can disentangle different dynamical scales. Integrating out $P^z$ allows to connect quasi-DAs to QCD LCDAs, and then integrating out $m_H$ enables to relate QCD LCDAs to HQET LCDAs. To verify this proposal, we make use of lattice QCD simulation on a lattice ensemble with spacing $a = 0.05187\,\mathrm{fm}$. The preliminary findings for HQET LCDAs qualitatively align with phenomenological models. Using a recent model for HQET LCDAs, we also fit the first inverse moment $\lambda_B^{-1}$ and the result is consistent with the experimentally constrain from $B \to \gamma \ell \nu_\ell$. This agreement demonstrates the promise of our method in providing first-principle predictions for heavy meson LCDAs.

*Introduction:* Weak decays of heavy mesons provide an excellent laboratory to test the Standard Model of particle physics, search for new physics phenomena beyond, and refine our understanding of the strong and weak nuclear forces. Theoretical predictions on rates of heavy meson decays based on QCD factorization theorems [1–4] hinge critically on the knowledge of heavy meson lightcone distribution amplitudes (LCDAs) defined in heavy quark effetive theory (HQET). The LCDAs encode the information about the probabilities of finding the quark and antiquark carrying certain momentum inside heavy meson [5]. In addition they are essential for understanding the dynamics of the strong force at the interface between the long-range hadronic properties and the short-range quark-gluon degrees of freedom.

Though the ultraviolet behavior is understandable from QCD perturbation theory [6–11], establishing a reliable result on the full distribution of heavy meson LCDAs is extremely difficult due to various reasons. Using experimental data to constrain LCDAs is challenging due to the intricate nature of heavy meson decay amplitudes. The strong interaction between quarks and gluons is nonperturbative at low energies, making it difficult to calculate the distribution amplitudes analytically. This nonperturbative behavior requires sophisticated theoretical frameworks to study the distribution amplitudes quantitatively. Constructing models or parameterizations involves assumptions about the internal structure of heavy mesons, and the choice of model will unavoidably introduce uncertainties and biases. Performing the lattice QCD calculation of heavy meson LCDAs directly is known to be complicated by the appearance of the lightcone separated quark fields defining the HQET matrix element for a long time. Defined by HQET fields, heavy meson LCDAs do not have well-defined non-negative moments due to the existence of cusp divergences [12], and thus it is not possible to calculate moments of heavy meson LCDAs as in the light meson case. Earlier attempts to use HQET equal-time correlators [13–19] are not easy to be implemented on the lattice.

In this Letter, we propose a sequential matching method to determine heavy meson LCDAs from lattice QCD. We employ the equal-time correlation functions, also named as quasi distribution amplitudes (quasi-DAs), of heavy meson with a large momentum component $P^z$. There are three energy scales in the correlation function which satisfies a hierarchical ordering $P^z \gg m_H \gg \Lambda_{\mathrm{QCD}}$. We point out that dynamics in these scales can be separated by integrating out the $P^z$ and $m_H$ in two steps. Integrating out the $P^z$, one can match the quasi-DAs onto QCD LCDAs, which is conducted in large momentum effective theory (LaMET) [20, 21] (see Ref. [22, 23] for recent reviews). After integrating out the $m_H$, one can match the QCD LCDAs onto boosted HQET and obtain the required LCDAs in HQET. To verify this proposal, we perform a lattice QCD simulation of quasi-DAs on a lattice ensemble with $a = 0.05187\,\text{fm}$. Our preliminary findings for HQET LCDAs qualitatively align with the existing phenomenological models. Using a recent model for HQET LCDAs, we also fit the first inverse moment and the obtained result $\lambda_B = 0.449\,(42)\,\text{GeV}$ lies in the experimentally constrained region $\lambda_B > 0.24\,\text{GeV}$ derived from $B \to \gamma\ell\nu_\ell$ measurement [24]. The overall agreement demonstrates the promise of our method in providing first-principle predictions for heavy meson LCDAs.

*Theoretical method:* The leading-twist LCDA for heavy meson encodes the information on the momentum distribution of the light-quark in heavy meson, and is essential for calculating various observables in heavy meson physics. In HQET, it can be defined as the Fourier transformation of the matrix element of a light-ray quark-gluon operator [12]

$$\varphi^+(\omega,\mu) = \frac{1}{i\tilde{f}_H(\mu)m_H}\int_{-\infty}^{+\infty}\frac{d\eta}{2\pi}\,e^{i\omega n_+\cdot v\eta} \\ \times \langle 0\,|\bar{q}(\eta n_+)\not{n}_+\gamma_5 W_c(\eta n_+,0)h_v(0)|\,H(v)\rangle\ , \qquad (1)$$

where $\omega$ denotes the momentum of the light quark. $n_+$ denotes the light-cone unit vector with $n_+^2 = 0$, $v_\mu$ is the heavy quark velocity satisfying $v^2 = 1$. $|H(v)\rangle$ is the heavy meson state with mass $m_H$. $\tilde{f}_H(\mu)$ signifies the static decay constant of heavy meson in HQET. $W_c(\eta n_+,0) = P\exp\left[ig_s\int_0^\eta dx\,n_+\cdot A(xn_+)\right]$ denotes the Wilson line to ensure the gauge invariance of the matrix element.

In order to obtain the desired LCDA $\varphi^+(\omega,\mu)$, we propose to utilize quasi distribution amplitude defined as

$$\tilde{\phi}(x,P^z;m_H) = \int\frac{dz}{2\pi}e^{-ixP^z z}\frac{\tilde{M}^0(z,P^z;\gamma^z\gamma_5,m_H)}{\tilde{M}^0(z,0;\gamma^t\gamma_5,m_H)}\,, \qquad (2)$$

where $P^z$ denotes the momentum along the $z$ direction. The involved matrix element is defined as

$$\tilde{M}^0(z,P^z;\Gamma,m_H) = \langle 0\,|\bar{q}(z)\Gamma W_c(z,0)Q(0)|\,H(P^z)\rangle\ . \qquad (3)$$

Here the $\tilde{M}^0(z,0;\gamma^t\gamma_5,m_H)$ in denominator of Eq. (2) is used to renormalize the bare matrix element $\tilde{M}^0(z,P^z;\Gamma,m_H)$.

An advantage of the quasi-DA is that it is an equal-time correlation and can be directly simulated on the lattice. On the other side, in large momentum limit, the quasi-DA involves three characteristic scales $P^z$, $m_H$ and $\Lambda_{\text{QCD}}$, for which we choose a hierarchical ordering $P^z \gg m_H \gg \Lambda_{\text{QCD}}$. With this hierarchy, the first two energy scales are within the perturbative regime and can be successively integrated out. In the first step, one can integrate out $P^z$ enabling the matching of the quasi DA to LCDA defined in terms of QCD quark-gluon fields. This procedure aligns with the treatment of parton distribution functions (PDFs) and light meson LCDAs in LaMET (for recent progress please see reviews [22, 23]). Once the QCD LCDA is obtained, the next step involves integrating out the $m_H$ scale and matching the quantities onto the boosted HQET. This procedure allows for the derivation of LCDAs in HQET.

More specifically, in the framework of LaMET, there is a factorization formula for quasi-DA once integrating out the momentum of heavy meson $P^z$

$$\tilde{\phi}(x,P^z;m_H) = \int_0^1 C\left(x,y,\frac{\mu}{P^z}\right)\phi(y,\mu;m_H) \\ +\mathcal{O}\left(\frac{m_H^2}{(P^z)^2},\frac{\Lambda_{\text{QCD}}^2}{(xP^z,\bar{x}P^z)^2}\right), \qquad (4)$$

where $\bar{x} = 1-x$, and $\phi(y;\mu,m_H)$ is the LCDA for heavy meson in QCD and defined as

$$\phi(y,\mu;m_H) = \frac{1}{if_H}\int_{-\infty}^{+\infty}\frac{d\tau}{2\pi}\,e^{iyP_H\tau n_+} \\ \times \langle 0\,|\bar{q}(\tau n_+)\not{n}_+\gamma_5 W_c(\tau n_+,0)Q(0)|\,H(P_H)\rangle\ . \qquad (5)$$

where $Q$ is the heavy quark field in QCD, $f_H$ is the decay constant in QCD. The difference between $f_H$ and $\tilde{f}_H$ is perturbatively calculable [5, 6]. The scale $\mu$ in the above satisfies $m_H < \mu < P^z$, and using the renormalization group equation one can evolve the LCDAs from $\mu = P^z$ to $\mu = m_H$.

The matching coefficient in Eq. (4) up to $\mathcal{O}(\alpha_s)$ is

$$C\left(x,y,\frac{\mu}{P^z}\right) = \delta(x-y) + C_B^{(1)}\left(x,y,\frac{\mu}{P^z}\right) - C_{CT}^{(1)}(x,y)\ , \qquad (6)$$

with $C_B^{(1)}$ calculated in [25]. The counter-term $C_{CT}^{(1)}$ comes from contribution of zero-momentum matrix element $\tilde{M}^0(z,0;\gamma^t\gamma_5,m_H)$ and its one loop result is derived as

$$C_{CT}^{(1)}(x,y) = -\frac{3\alpha_s C_F}{4\pi}\left|\frac{1}{x-y}\right|_+ . \qquad (7)$$

Once having $\phi(y;\mu,m_H)$ at hand, one can further integrate out the large $m_H$ scale, which is valid when $m_H \gg \Lambda_{\text{QCD}}$ [26–28]. This will lead to a factorization of QCD LCDAs:

$$\phi\,(y,\mu;m_H) = \frac{\tilde{f}_H}{f_H}J_{\text{peak}}m_H\varphi^+(\omega,\mu) + \mathcal{O}\left(\frac{\Lambda_{\text{QCD}}}{m_H}\right)\,, \qquad (8)$$

where $\omega = y m_H$. This factorization is multiplicative and the one-loop matching kernel $J_{\text{peak}}$ can be found in Ref. [28]. The scale $\mu$ here satisfies $\Lambda_{\text{QCD}} < \mu < m_H$, and the renormalization group equation allows to evolve the HQET LCDAs to a low energy scale.

It is worth noting that in HQET the momentum of a light quark is typically soft. Therefore, the factorization in the second step only works in the region with $\omega \sim \Lambda_{\text{QCD}}$, named as peak region. In contrast, when the momentum of the light quark is large with $\omega \gg \Lambda_{\text{QCD}}$ or $y \sim 1$, the heavy quark will carry a relatively small momentum. This is referred to as tail region, and in this region, the LCDA is perturbative. Thereby it can be handled using QCD perturbation theory, and the one-loop result can be found in Ref. [7]. Once the results in the two distinct regions are obtained, they can be combined to construct a complete distribution for the LCDA in HQET.

In LaMET, introducing quasi-DAs with a finite but large $P^z$ offers a great advantage of enabling direct lattice calculations, thus circumventing the challenges associated with accessing the lightcone directly [20, 21]. Our method follows a similar methodology. Specifically, when considering an infinitely heavy quark mass, the utilization of heavy quark field in HQET is hindered by limitations of lattice implementation. To address this obstacle, we have constructed the quasi-DAs incorporating a finite heavy quark mass and a large $P^z$, facilitating direct simulations and subsequent matching onto the final HQET LCDAs.

*Lattice QCD verification:* To verify our proposal, we will conduct a lattice QCD simulation using configurations characterized by a spacing of $a = 0.05187\,\text{fm}$ and a box length of $L = 48\,a \simeq 2.5\,\text{fm}$. These ensembles were recently generated with $2+1$ flavor stout smeared clover fermions and Symanzik gauge action as outlined in Ref. [29], and have been successfully applied in studies involving hadron spectrum [30, 31], decay and mixing of charmed hadron [32–34] and other interesting phenomena [35, 36]. On this ensemble, the valence light quark parameter is chosen such that the pion mass is approximately 317 MeV. To maintain the hierarchical ordering $P^z \gg m_H \gg \Lambda_{\text{QCD}}$, we opt to focus on simulating the $D$ meson. The charm quark mass on the lattice is adjusted to reproduce the physical mass of $J/\psi$, resulting in a calculated $D$ meson mass on this lattice ensemble of $m_D \simeq 1.92\,\text{GeV}$. Utilizing a dataset of 549 gauge configurations, we perform 32 measurements of quasi matrix elements on each configuration with boosted momenta $P^z$ reaching up to $16\pi/L \simeq 3.98\,\text{GeV}$. The pertinent dispersion relation is collected in supplemental material.

We construct the nonlocal two-point correlation function as

$$C_2^{\Gamma}(z, P^z, t) = \sum_{\vec{x}} \operatorname{Tr} e^{iP^z z} \times \left\langle S_q^{\dagger}(\vec{x} + z\hat{n}_z, t; 0)\gamma_5 \Gamma W_c(\vec{x} + z\hat{n}_z, \vec{x}) S_Q(\vec{x}, t; 0)\right\rangle , \tag{9}$$

where $S_q/S_Q$ is the light/heavy quark propagator from a Coulomb gauge fixed grid source to point sink. The relation $\gamma_5 S_q^{\dagger}(y, x)\gamma_5 = S_q(x, y)$ have been applied for the antiquark propagator. We choose the $\Gamma = \gamma^z\gamma_5$ for the matrix elements with nonzero momentum in Eq. (2) and $\Gamma = \gamma^t\gamma_5$ for those with zero momentum.

Based on the reduction formula for the two-point function, one can determine $\tilde{M}_{\Gamma}^0(z, P^z) \equiv \tilde{M}^0(z, P^z; \Gamma, m_D)$ through a correlated joint fit of the following ratio:

$$\frac{C_2^{\Gamma}(z, P^z, t)}{C_2^{\Gamma}(0, P^z, t)} = \tilde{M}_{\Gamma}^0(z, P^z)\frac{1 + c_z e^{-\Delta E_z t}}{1 + c_0 e^{-\Delta E_0 t}} . \tag{10}$$

where the parameters $c_0$, $c_z$ and $\Delta E_0$, $\Delta E_z$ correspond to contamination from excited states. The $\tilde{M}^0_{\gamma^z\gamma_5}(z, P^z)/\tilde{M}^0_{\gamma^t\gamma_5}(z, 0)$ as a function of $\lambda = zP^z$ is depicted in Fig. 1 at $P^z = \{2.99,\, 3.49,\, 3.98\}\,\text{GeV}$, respectively. Both the real and imaginary parts exhibit decaying behavior with oscillatory and become uncertain as $\lambda$ increases.

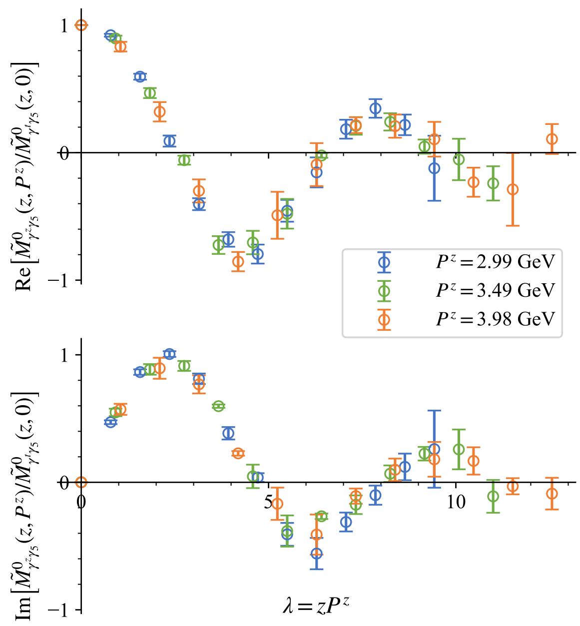


FIG. 1. Results for the renormalized matrix elements $\tilde{M}^0_{\gamma^z\gamma_5}(z, P^z)/\tilde{M}^0_{\gamma^t\gamma_5}(z, 0)$ as function of $\lambda = zP^z$ with $P^z = \{2.99,\, 3.49,\, 3.98\}\,\text{GeV}$.

To reduce the fluctuations at large $\lambda$ within quasi-DA, we extrapolate the above results based on an extrapolation model [37]. In practice, we adopt the renormalized matrix elements at $z \geq 8\,a$ for the extrapolation fit and to reconstruct the distributions that characterize the long-distance behavior.

We then Fourier transform the matrix elements to the momentum space, and subsequently match to the QCD LCDA using the matching formula provided in Eq. (4) [38–43]. Fig. 2 displays the results for QCD LCDA with three different momenta $P^z = \{2.99, 3.49, 3.98\}$ GeV. All distributions exhibit a peak in the small-$x$ region due to the tendency of light quark to have a smaller momentum fraction. In LaMET, it is preferable to have a large momentum in order to suppress power corrections, and the final results can be obtained once the convergence is achieved. From the figure, we observe a trend towards convergence at $P^z$ around $3 \sim 4$ GeV, with a corresponding boosting factor of $\gamma \sim 2$. As an attempt, we employ the result at $P^z = 3.98$ GeV for the following analysis.

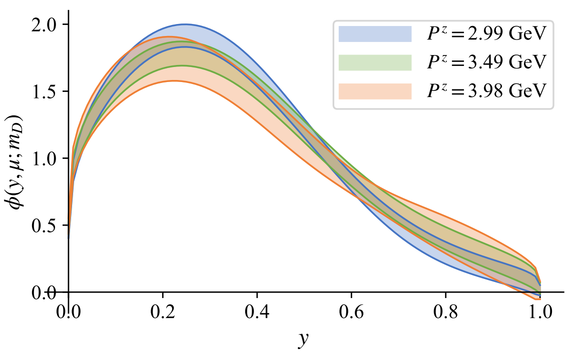


FIG. 2. The $P^z$ dependence of heavy meson QCD LCDA at scale $\mu = 2$ GeV. The bands are consistent with each other within errors.

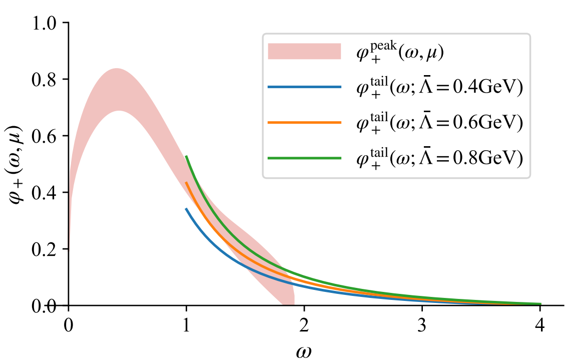


FIG. 3. Peak and tail region of HQET LCDA. The peak region is extracted from lattice QCD calculation and the tails is solved perturbatively at one-loop order with different $\bar{\Lambda}$.

As noted previously, in the peak region where the light quark momentum fraction $y$ is at $\mathcal{O}(\Lambda_{\mathrm{QCD}}/m_H)$, the QCD LCDA can be matched to the HQET LCDA with the multiplicative formula in Eq. (8). The corresponding outcome is shown as the pink band in Fig. 3.

While in the tail region, the HQET LCDA is perturbatively calculable. We employ the one-loop level result [7]:

$$\varphi^+_{\mathrm{tail}}(\omega, \mu) = \frac{\alpha_s C_F}{\pi \omega} \left[ \left( \frac{1}{2} - \ln \frac{\omega}{\mu} \right) + \frac{4\bar{\Lambda}}{3\omega} \left( 2 - \ln \frac{\omega}{\mu} \right) \right] , \tag{11}$$

in which the parameter $\bar{\Lambda} = m_H - m_Q$ denotes the effective light quark mass which is typically about hundreds of MeV. In Fig. 3, we show this result with $\bar{\Lambda} = \{0.4, 0.6, 0.8\}$ GeV.

In Fig. 3, the $\varphi^+_{\mathrm{tail}}(\omega, \bar{\Lambda} = 0.4\,\mathrm{GeV})$ and $\varphi^+_{\mathrm{tail}}(\omega, \bar{\Lambda} = 0.8\,\mathrm{GeV})$ intersect with lattice results at $\omega$ around $1.5 \sim 1.8$ GeV. These values significantly exceed the nonperturbative scale $\bar{\Lambda}$. By combining the lattice results in peak region with the perturbative result in tail region with $\omega \in [1.5, 1.8]$ GeV, and smoothing the junction using a polynomial filter, we arrive at the final outcome represented by the pink band in Fig. 4.

As a comparison, we show in Fig. 4 several phenomenological models for HQET LCDAs [44–46]:

$$\begin{aligned}
\varphi^+_{\mathrm{I}}(\omega, \mu_0) &= \frac{\omega}{\omega_0^2} e^{-\omega/\omega_0} , \\
\varphi^+_{\mathrm{II}}(\omega, \mu_0) &= \frac{4}{\pi \omega_0} \frac{k}{k^2+1} \left[ \frac{1}{k^2+1} - \frac{2\left(\sigma_B^{(1)} - 1\right)}{\pi^2} \ln k \right] , \\
\varphi^+_{\mathrm{III}}(\omega, \mu_0) &= \frac{2\omega^2}{\omega_0 \omega_1^2} e^{-(\omega/\omega_1)^2} , \\
\varphi^+_{\mathrm{IV}}(\omega, \mu_0) &= \frac{\omega}{\omega_0 \omega_2} \frac{\omega_2 - \omega}{\sqrt{\omega(2\omega_2 - \omega)}} \theta(\omega_2 - \omega) , \\
\varphi^+_{\mathrm{V}}(\omega, \mu_0) &= \frac{\Gamma(\beta)}{\Gamma(\alpha)} \frac{\omega}{\omega_0^2} e^{-\omega/\omega_0} U(\beta - \alpha, 3 - \alpha, \omega/\omega_0) ,
\end{aligned} \tag{12}$$

where $\omega_0 = 350$ MeV, $\omega_1 = 2\omega_0/\sqrt{\pi}$, $\omega_2 = 4\omega_0/(4-\pi)$, and $k = \omega/1$ GeV. In model V, $U(a, b, z)$ denotes the second kind confluent hypergeometric function, and the parameters $\alpha$ and $\beta$ can be found in Ref. [45, 46]. In Fig. 4, it is evident that all phenomenological models exhibit a peak distribution at $\omega \approx 0.4$ GeV, yet they vary notably in shape. Model II, III, and IV deviate from the perturbative constraint as $\omega$ approaches infinity. Our findings align with these models on a qualitative level, notably demonstrating good agreement with model V, which integrates the constraint through renormalization group equation and analyticity principles.

At leading power in $m_H$, the first inverse moment $\lambda_B^{-1}$ of HQET LCDA governs the decay rate of $B \to \gamma \ell \nu$ with an energetic photon (energy $E_\gamma$) in the final state. Thereby we also extract the first inverse moment from our result. Since our result has a similar shape with model V, we fit the parameter in this model with $\omega \in [0.2, 1.5]$ GeV. Using the fitted parameter, we obtain the

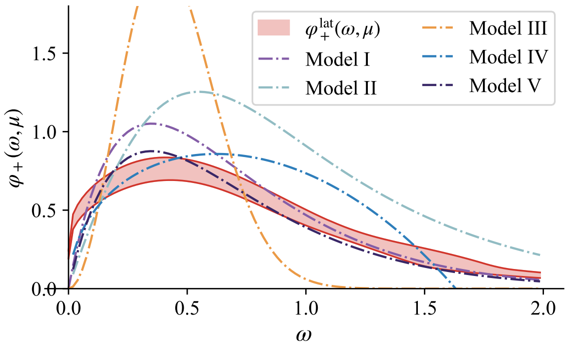


FIG. 4. Preliminary results on $\varphi^+(\omega,\mu)$ and its comparison with phenomenological models. Error in the lattice result is statistical only.

result:

$$\lambda_B = 0.449(42)\,\mathrm{GeV}. \tag{13}$$

The available data from Belle collaboration gives an lower bound $\lambda_B > 0.24\,\mathrm{GeV}$ at 90% confidence level [24]. Our obtained result is also in accordance with the phenomenological calculations in Refs. [5, 7, 12, 47]. More comparison and discussions can be found in the supplemental material. The overall agreement demonstrates the promise of our method in providing first-principles predictions for heavy meson LCDAs.

*Summary and prospect:* In this Letter, we have presented a first-principle method for calculating the leading-twist HQET LCDA of heavy mesons. We have developed lattice QCD computable quasi-DAs characterized by three distinct dynamical scales arranged in a hierarchical order $P^z \gg m_H \gg \Lambda_{\mathrm{QCD}}$. It is demonstrated that the separation of various dynamical scales can be achieved sequentially through a two-step factorization process. Within LaMET, we integrate out the $P^z$ and match the quasi-DAs onto QCD LCDAs. Subsequently, the HQET LCDAs can be obtained by integrating out the heavy meson scale $m_H$. One benefit of this method is the elimination of the need to simulate the HQET heavy quark field on the lattice.

To validate this approach, we have conducted lattice QCD simulations of $D$ meson quasi-DA on a single ensemble with $a = 0.05187\,\mathrm{fm}$ as an attempt and successfully matched it to the HQET LCDA. Our findings, though preliminary, exhibit qualitative agreement with several established phenomenological models. Through fitting the parameter in the latest model, we have also extracted the first inverse moment $\lambda_B = 0.449\,(42)\,\mathrm{GeV}$, which lies in the experimentally constrained region derived from $B \to \gamma\ell\nu_\ell$ measurement.

Despite of the encouraging finding, further improvements are necessary. It is crucial to recognize that all results presented in this study are subject to statistical uncertainties. To achieve better precision, it is imperative to address systematic effects. Potential sources of systematic uncertainties that can be improved upon in the next stage include the following.

- For the simulation, a comprehensive lattice QCD calculation across multiple ensembles featuring different lattice spacings and pion masses is needed. Smaller lattice spacings will offer a wider range of $P^z$ values, enhancing the effectiveness of the hierarchy across the three scales and facilitating tighter control over power corrections during the matching process. A more robust nonperturbative renormalization in such as hybrid scheme [37, 48] is essential, and operator mixing effects must be carefully considered.

- Aside from the improvement in lattice simulation, it is essential to appropriately deal with power corrections during the two-step matching process. Power corrections in terms of $m_H^2/(P^z)^2$ or $\Lambda_{\mathrm{QCD}}/m_H$ can be reduced by analysing higher twist contributions [49, 50], while those in terms of $\Lambda_{\mathrm{QCD}}^2/(xP^z, \bar{x}P^z)^2$ at the endpoint region of QCD LCDAs can be improved by RG resummation of the matching kernel and the inclusion of the renormalons effects. Furthermore, there is a pressing need for calculating higher-order perturbative corrections to the short-distance Wilson coefficient. These advancements are crucial for achieving precise determinations of the low-momentum characteristics of the HQET LCDAs. In addition, we have employed a straightforward method to merge the peak and tail regions, but a more dependable strategy is required to minimize potential uncertainties.

It is anticipated by incorporating these improvements in future our methodology will deliver reliable and accurate predictions on LCDAs and related quantities such as shape function of heavy meson from first-principles of QCD, and facilitate precise calculations for decay rates of heavy meson.

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[1] M. Beneke, G. Buchalla, M. Neubert and C. T. Sachrajda, Phys. Rev. Lett. **83**, 1914-1917 (1999) doi:10.1103/PhysRevLett.83.1914 [arXiv:hep-ph/9905312 [hep-ph]].

[2] M. Beneke, G. Buchalla, M. Neubert and C. T. Sachrajda, Nucl. Phys. B **591**, 313-418 (2000) doi:10.1016/S0550-3213(00)00559-9 [arXiv:hep-ph/0006124 [hep-ph]].

[3] Y. Y. Keum, H. N. Li and A. I. Sanda, Phys. Rev. D **63**, 054008 (2001) doi:10.1103/PhysRevD.63.054008 [arXiv:hep-ph/0004173 [hep-ph]].

[4] C. D. Lu, K. Ukai and M. Z. Yang, Phys. Rev. D **63**, 074009 (2001) doi:10.1103/PhysRevD.63.074009 [arXiv:hep-ph/0004213 [hep-ph]].

[5] A. G. Grozin and M. Neubert, Phys. Rev. D **55**, 272-290 (1997) doi:10.1103/PhysRevD.55.272 [arXiv:hep-ph/9607366 [hep-ph]].

[6] B. O. Lange and M. Neubert, Phys. Rev. Lett. **91**, 102001 (2003) doi:10.1103/PhysRevLett.91.102001 [arXiv:hep-ph/0303082 [hep-ph]].

[7] S. J. Lee and M. Neubert, Phys. Rev. D **72**, 094028 (2005) doi:10.1103/PhysRevD.72.094028 [arXiv:hep-ph/0509350 [hep-ph]].

[8] H. Kawamura and K. Tanaka, Phys. Lett. B **673**, 201-207 (2009) doi:10.1016/j.physletb.2009.02.028 [arXiv:0810.5628 [hep-ph]].

[9] G. Bell, T. Feldmann, Y. M. Wang and M. W. Y. Yip, JHEP **11**, 191 (2013) doi:10.1007/JHEP11(2013)191 [arXiv:1308.6114 [hep-ph]].

[10] T. Feldmann, B. O. Lange and Y. M. Wang, Phys. Rev. D **89**, no.11, 114001 (2014) doi:10.1103/PhysRevD.89.114001 [arXiv:1404.1343 [hep-ph]].

[11] V. M. Braun, Y. Ji and A. N. Manashov, Phys. Rev. D **100**, no.1, 014023 (2019) doi:10.3204/PUBDB-2019-02451 [arXiv:1905.04498 [hep-ph]].

[12] V. M. Braun, D. Y. Ivanov and G. P. Korchemsky, Phys. Rev. D **69**, 034014 (2004) doi:10.1103/PhysRevD.69.034014 [arXiv:hep-ph/0309330 [hep-ph]].

[13] H. Kawamura and K. Tanaka, PoS **RADCOR2017**, 076 (2018) doi:10.22323/1.290.0076

[14] W. Wang, Y. M. Wang, J. Xu and S. Zhao, Phys. Rev. D **102**, no.1, 011502 (2020) doi:10.1103/PhysRevD.102.011502 [arXiv:1908.09933 [hep-ph]].

[15] S. Zhao and A. V. Radyushkin, Phys. Rev. D **103**, no.5, 054022 (2021) doi:10.1103/PhysRevD.103.054022 [arXiv:2006.05663 [hep-ph]].

[16] J. Xu, X. R. Zhang and S. Zhao, Phys. Rev. D **106**, no.1, L011503 (2022) doi:10.1103/PhysRevD.106.L011503 [arXiv:2202.13648 [hep-ph]].

[17] J. Xu and X. R. Zhang, Phys. Rev. D **106**, no.11, 114019 (2022) doi:10.1103/PhysRevD.106.114019 [arXiv:2209.10719 [hep-ph]].

[18] S. M. Hu, W. Wang, J. Xu and S. Zhao, Phys. Rev. D **109**, no.3, 034001 (2024) doi:10.1103/PhysRevD.109.034001 [arXiv:2308.13977 [hep-ph]].

[19] S. M. Hu, J. Xu and S. Zhao, [arXiv:2401.04291 [hep-ph]].

[20] X. Ji, Phys. Rev. Lett. **110**, 262002 (2013) doi:10.1103/PhysRevLett.110.262002 [arXiv:1305.1539 [hep-ph]].

[21] X. Ji, Sci. China Phys. Mech. Astron. **57**, 1407-1412 (2014) doi:10.1007/s11433-014-5492-3 [arXiv:1404.6680 [hep-ph]].

[22] X. Ji, Y. S. Liu, Y. Liu, J. H. Zhang and Y. Zhao, Rev. Mod. Phys. **93**, no.3, 035005 (2021) doi:10.1103/RevModPhys.93.035005 [arXiv:2004.03543 [hep-ph]].

[23] K. Cichy and M. Constantinou, Adv. High Energy Phys. **2019**, 3036904 (2019) doi:10.1155/2019/3036904 [arXiv:1811.07248 [hep-lat]].

[24] M. Gelb *et al.* [Belle], Phys. Rev. D **98**, no.11, 112016 (2018) doi:10.1103/PhysRevD.98.112016 [arXiv:1810.12976 [hep-ex]].

[25] Y. S. Liu, W. Wang, J. Xu, Q. A. Zhang, S. Zhao and Y. Zhao, Phys. Rev. D **99**, no.9, 094036 (2019) doi:10.1103/PhysRevD.99.094036 [arXiv:1810.10879 [hep-ph]].

[26] S. Ishaq, Y. Jia, X. Xiong and D. S. Yang, Phys. Rev. Lett. **125**, no.13, 132001 (2020) doi:10.1103/PhysRevLett.125.132001 [arXiv:1905.06930 [hep-ph]].

[27] S. Zhao, Phys. Rev. D **101**, no.7, 071503 (2020) doi:10.1103/PhysRevD.101.071503 [arXiv:1910.03470 [hep-ph]].

[28] M. Beneke, G. Finauri, K. K. Vos and Y. Wei, JHEP **09**, 066 (2023) doi:10.1007/JHEP09(2023)066 [arXiv:2305.06401 [hep-ph]].

[29] Z. C. Hu *et al.* [CLQCD], Phys. Rev. D **109**, no.5, 054507 (2024) doi:10.1103/PhysRevD.109.054507 [arXiv:2310.00814 [hep-lat]].

[30] H. Liu, J. He, L. Liu, P. Sun, W. Wang, Y. B. Yang and Q. A. Zhang, Sci. China Phys. Mech. Astron. **67**, no.1, 211011 (2024) doi:10.1007/s11433-023-2205-0 [arXiv:2207.00183 [hep-lat]].

[31] H. Xing, J. Liang, L. Liu, P. Sun and Y. B. Yang, [arXiv:2210.08555 [hep-lat]].

[32] Q. A. Zhang, J. Hua, F. Huang, R. Li, Y. Li, C. Lü, C. D. Lu, P. Sun, W. Sun and W. Wang, *et al.* Chin. Phys. C **46**, no.1, 011002 (2022) doi:10.1088/1674-1137/ac2b12 [arXiv:2103.07064 [hep-lat]].

[33] H. Liu, L. Liu, P. Sun, W. Sun, J. X. Tan, W. Wang, Y. B. Yang and Q. A. Zhang, Phys. Lett. B **841**, 137941 (2023) doi:10.1016/j.physletb.2023.137941 [arXiv:2303.17865 [hep-lat]].

[34] H. Liu, W. Wang and Q. A. Zhang, Phys. Rev. D **109**, no.3, 036037 (2024) doi:10.1103/PhysRevD.109.036037 [arXiv:2309.05432 [hep-ph]].

[35] D. J. Zhao *et al.* [$\chi$QCD], Phys. Rev. D **107**, no.9, L091501 (2023) doi:10.1103/PhysRevD.107.L091501 [arXiv:2207.14132 [hep-lat]].

[36] X. L. Meng *et al.* [$\chi$QCD and CLQCD], [arXiv:2305.09459 [hep-lat]].

[37] X. Ji, Y. Liu, A. Schäfer, W. Wang, Y. B. Yang, J. H. Zhang and Y. Zhao, Nucl. Phys. B **964**, 115311 (2021) doi:10.1016/j.nuclphysb.2021.115311 [arXiv:2008.03886 [hep-ph]].

[38] J. H. Zhang, J. W. Chen, X. Ji, L. Jin and H. W. Lin, Phys. Rev. D **95**, no.9, 094514 (2017) doi:10.1103/PhysRevD.95.094514 [arXiv:1702.00008

[hep-lat]].
[39] J. H. Zhang *et al.* [LP3], Nucl. Phys. B **939**, 429-446 (2019) doi:10.1016/j.nuclphysb.2018.12.020 [arXiv:1712.10025 [hep-ph]].
[40] H. W. Lin, J. W. Chen, Z. Fan, J. H. Zhang and R. Zhang, Phys. Rev. D **103**, no.1, 014516 (2021) doi:10.1103/PhysRevD.103.014516 [arXiv:2003.14128 [hep-lat]].
[41] R. Zhang, C. Honkala, H. W. Lin and J. W. Chen, Phys. Rev. D **102**, no.9, 094519 (2020) doi:10.1103/PhysRevD.102.094519 [arXiv:2005.13955 [hep-lat]].
[42] J. Hua *et al.* [Lattice Parton], Phys. Rev. Lett. **127**, no.6, 062002 (2021) doi:10.1103/PhysRevLett.127.062002 [arXiv:2011.09788 [hep-lat]].
[43] J. Hua *et al.* [Lattice Parton], Phys. Rev. Lett. **129**, no.13, 132001 (2022) doi:10.1103/PhysRevLett.129.132001 [arXiv:2201.09173 [hep-lat]].
[44] Y. M. Wang and Y. L. Shen, Nucl. Phys. B **898**, 563-604 (2015) doi:10.1016/j.nuclphysb.2015.07.016 [arXiv:1506.00667 [hep-ph]].
[45] M. Beneke, V. M. Braun, Y. Ji and Y. B. Wei, JHEP **07**, 154 (2018) doi:10.1007/JHEP07(2018)154 [arXiv:1804.04962 [hep-ph]].
[46] J. Gao, T. Huber, Y. Ji, C. Wang, Y. M. Wang and Y. B. Wei, JHEP **05**, 024 (2022) doi:10.1007/JHEP05(2022)024 [arXiv:2112.12674 [hep-ph]].
[47] A. Khodjamirian, R. Mandal and T. Mannel, JHEP **10**, 043 (2020) doi:10.1007/JHEP10(2020)043 [arXiv:2008.03935 [hep-ph]].
[48] Y. K. Huo *et al.* [Lattice Parton Collaboration (LPC)], Nucl. Phys. B **969**, 115443 (2021) doi:10.1016/j.nuclphysb.2021.115443 [arXiv:2103.02965 [hep-lat]].
[49] J. W. Chen, S. D. Cohen, X. Ji, H. W. Lin and J. H. Zhang, Nucl. Phys. B **911**, 246-273 (2016) doi:10.1016/j.nuclphysb.2016.07.033 [arXiv:1603.06664 [hep-ph]].
[50] W. Y. Liu and J. W. Chen, Phys. Rev. D **104**, no.9, 094501 (2021) doi:10.1103/PhysRevD.104.094501 [arXiv:2010.06623 [hep-ph]].
[51] R. G. Edwards *et al.* [SciDAC, LHPC and UKQCD], Nucl. Phys. B Proc. Suppl. **140**, 832 (2005) doi:10.1016/j.nuclphysbps.2004.11.254 [arXiv:hep-lat/0409003 [hep-lat]].
[52] M. A. Clark *et al.* [QUDA], Comput. Phys. Commun. **181**, 1517-1528 (2010) doi:10.1016/j.cpc.2010.05.002 [arXiv:0911.3191 [hep-lat]].
[53] R. Babich *et al.* [QUDA], doi:10.1145/2063384.2063478 [arXiv:1109.2935 [hep-lat]].
[54] M. A. Clark *et al.* [QUDA], doi:10.5555/3014904.3014995 [arXiv:1612.07873 [hep-lat]].
[55] Y. J. Bi, Y. Xiao, W. Y. Guo, M. Gong, P. Sun, S. Xu and Y. B. Yang, PoS **LATTICE2019**, 286 (2020) doi:10.22323/1.363.0286 [arXiv:2001.05706 [hep-lat]].

## SUPPLEMENTAL MATERIALS

### A. Dispersion relation

The effective energies of heavy mesons can be determined from the local two-point correlation function. By substituting $z = 0$ into Eq. (3), we can fit the effective energies using a parametrization of the correlation functions. This analysis allows for the examination of the dispersion relation of the heavy meson. In Fig. 5, the data points represent the effective energies of the $D$ meson up to $P = 16\pi/L \simeq 3.98\,\text{GeV}$, while the curve illustrates the fit determined by the formula:

$$E^2 = m_D^2 + c_0 P^2 + c_1 P^4 a^2, \tag{14}$$

with fit results $m_D = 1.9151\,(57)\text{GeV}$, $c_0 = 1.007\,(30)$, and $c_1 = -0.142\,(45)$. The deviation of $c_0$ from unity and $c_1$ from null accounts for discretization errors.

### B. First inverse moment $\lambda_B^{-1}$

The first inverse moment is a crucial quantity in lightcone sum-rule studies and QCD factorization theorems in heavy flavor physics. While it has been estimated using various approaches, there remains significant room for improvement in reliability and precision. Therefore, investigating the first inverse moment on the lattice holds substantial phenomenological importance.

In this work, we fit our data based on the models in Eq. (12). The fitting outcomes, including the fit range and the corresponding $\chi^2$/d.o.f for each model, are summarized in Tab. I. Due to the distinct behavior of $\omega$ in model III, fit of our results using this model is inappropriate. Additionally, model IV does not encompass the tail region, leading us to use a narrower range of $\omega$ for the fitting process. It is worth noting that in these models, the parameter $\omega_0$ is equal to $\lambda_B$.

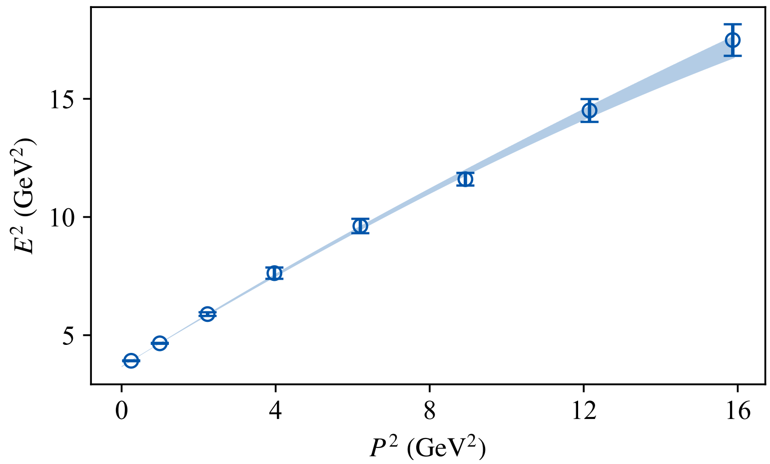


FIG. 5. The dispersion relation of $D$ meson with its effective energies extracted from the local two-point correlation function. The data up to $P = 16\pi/L \simeq 3.98\,\mathrm{GeV}$ are fitted using Eq. (14), yielding $m_D = 1.9151\,(57)$, $c_0 = 1.007\,(30)$ and $c_1 = -0.142\,(45)$.

TABLE I. Fit results based on each models in Eq. (12). Due to the distinct behavior of $\omega$, we unable to fit our result from model III.

| Models | I | II | III | IV | V |
|---|---|---|---|---|---|
| Parameters | $\omega_0 = 0.433(23)$GeV | $\omega_0 = 0.682(45)$GeV | —— | $\omega_0 = 0.427(21)$GeV | $\omega_0 = 0.449(42)$GeV |
| | | $\sigma_B^{(1)} = 2.78(48)$ | | | |
| fit range | $\omega \in [0.2, 1.4]$GeV | $\omega \in [0.2, 1.4]$GeV | | $\omega \in [0.4, 0.8]$GeV | $\omega \in [0.2, 1.4]$GeV |
| $\chi^2$/d.o.f | 1.4 | 1.2 | | 2.1 | 1.0 |

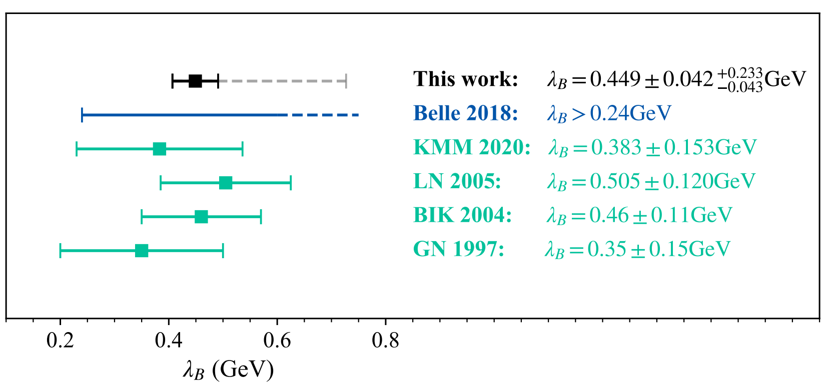


FIG. 6. The first inverse moment of heavy meson LCDA obtained in this work and from other phenomenological studies (KMM2020 [47], LN2005 [7], BIK2004 [12] and GN1997 [5], which are labeled in cyan). A lower bound (Blue) from Belle measurement of $B \to \gamma \ell \nu$ [24] is also provided. When displaying our findings, we have employed model V as default, with variations from other models depicted as gray dashed bands.