We study the scattering of light pseudoscalar mesons ($\pi, K$) off charmed mesons ($D, D_s$) in full lattice QCD. The $S$-wave scattering lengths are calculated using Lüscher’s finite volume technique. We use a relativistic formulation for the charm quark. For the light quark, we use domain-wall fermions in the valence sector and improved Kogut-Susskind sea quarks. We calculate the scattering lengths of isospin-3/2 $D\pi$, $D_s\pi$, $D_sK$, isospin-0 $D K$ and isospin-1 $D K$ channels on the lattice. For the chiral extrapolation, we use a chiral unitary approach to next-to-leading order, which at the same time allows us to give predictions for other channels. It turns out that our results support the interpretation of the $D_s^*(2317)$ as a $DK$ molecule. At the same time, we also update a prediction for the isospin breaking hadronic decay width $\Gamma(D_s^*(2317) \to D_s\pi)$ to $(133 \pm 22)$ keV.

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PACS numbers: 12.38.Gc, 12.39.Fe, 13.75.Lb, 14.40.Lb

I. INTRODUCTION

In 2003, the BABAR Collaboration discovered a positive-parity scalar charm-strange meson $D_s^*(2317)$ with a very narrow width [1]. The state was confirmed later by the CLEO Collaboration [2]. The discovery of this state has inspired heated discussions in the past decade. The key point is to understand the low mass of this state, which is more than 100 MeV lower than the prediction for its structure, such as being a $DK$ molecule, the chiral partner of the pseudoscalar $D_s$, a conventional $c\bar{s}$ state, coupled-channel effects between the $c\bar{s}$ state and $DK$ continuum etc. For a detailed review of the properties and the phenomenology of these states see Ref. [4]. In order to distinguish them, one has to explore the consequences of each interpretation, and identify quantities which have different values in different interpretations. Arguably the most promising quantity is the isospin breaking width $\Gamma(D_s^*(2317) \to D_s\pi)$. It is of order 10 keV if the $D_s^*(2317)$ is a $c\bar{s}$ meson [5,6], while it is of order 100 keV [7–9] in the $DK$ molecular picture due to its large coupling to $DK$ and the proximity of the $DK$ threshold.

Thus, the study of $DK$ interaction is very important in order to understand the structure of $D_s^*(2317)$ (a suggestion of studying this state in a finite volume was made in Ref. [10]). Although a direct simulation of the $DK(I = 0)$ channel suffers from disconnected diagrams, one may obtain useful information on the $DK$ interaction by calculating the scattering lengths of the disconnected-diagram-free channels which can be related to $DK(I = 0)$ through SU(3) flavor symmetry. This is the strategy we will follow in this paper.

Lattice QCD calculations of the properties of hadronic interactions such as elastic scattering phase shifts and scattering lengths have recently started to develop. Precision results have been obtained in the light meson sector for certain processes such as pion-pion, kaon-kaon and pion-kaon scattering and preliminary results for baryon-baryon scattering lengths have been presented. A review of these calculations can be found in Ref. [11]. In the heavy meson sector, only a few calculations have been done, including quenched calculations in Refs. [12,13] and calculations in full QCD in Refs. [14,15]. In this work, we study scattering processes where one of the hadrons contains a charm quark in full lattice QCD.

Extracting hadronic interactions from lattice QCD calculations is not straightforward due to the Maiani-Testa theorem [16], which states that the $S$ matrix cannot be extracted from infinite-volume Euclidean-space Green functions except at kinematic thresholds. However, this problem can be evaded by computing the correlation functions in a finite volume. Lüscher has shown that one can...
obtain the scattering amplitude from the energy of two particles in a finite volume [17,18]. We use Lüscher’s finite volume technique to calculate the scattering lengths. We then use unitarized chiral perturbation theory to extrapolate our results to the physical pion mass. Having fitted the appearing low-energy constants (LECs) to the lattice data, we are also able to make predictions for other channels, in particular for the isospin zero, strangeness one channel in which the \( D_s(2317) \) resides.

The paper is organized as follows. The lattice formulation of the light and heavy quark actions will be discussed in Sec. II. Lüscher’s formula will be briefly introduced in Sec. III. The numerical results for the scattering lengths of five channels \( D\bar{K}(I = 0), D\bar{K}(I = 1), D_s K, D\pi(I = 3/2) \) and \( D_s\pi \) which are free of disconnected diagrams will be given in Sec. IV. Chiral extrapolations will be performed using unitarized chiral perturbation theory in Sec. V, and values of the LECs in the chiral Lagrangian will be determined. Predictions for other channels using the LECs are given in Sec. VI, and in particular, implications on the \( D_s(2317) \) will be discussed. The last section is devoted to a brief summary.

II. LATTICE FORMULATION

A. Light-quark action

In this work we employ the “coarse” (\( a \approx 0.125 \) fm) gauge configurations generated by the MILC Collaboration [19] using the one-loop tadpole-improved gauge action [20], where both \( \mathcal{O}(a^2) \) and \( \mathcal{O}(g^2a^2) \) errors are removed. For the fermions in the vacuum, the asqtad-improved Kogut-Susskind (staggered) action [21–26] is used. This is the so-called Naik action [27] \( \mathcal{O}(a^3) \) improved Kogut-Susskind action with smeared links for the one-link terms so that couplings to gluons with any of their momentum components equal to \( \pi/a \) are set to zero, resulting in a reduction of the flavor symmetry violations present in the Kogut-Susskind action.

For the valence light quarks (up, down and strange) we use the five-dimensional Shamir [28,29] domain-wall fermion action [30]. The domain-wall fermion action introduces a fifth dimension of extent \( L_s \) and a mass parameter \( M_s \); in our case, the values \( L_s = 16 \) and \( M_s = 1.7 \), both in lattice units, were chosen. The physical quark fields, \( q(x,t) \), reside on the four-dimensional boundaries of the fifth coordinate. The left and right chiral components are separated on the corresponding boundaries, resulting in an action with chiral symmetry at finite lattice spacing as \( L_s \to \infty \). We use hypercubic-smeared gauge links [31–34] to minimize the residual chiral symmetry breaking, and the bare quark-mass parameter \( (am)_q^{\text{dwa}} \) is introduced as a direct coupling of the boundary chiral components. The light quark propagators were provided to us by the NPLQCD [11] and LHP [35–37] Collaborations.

The calculation we have performed, because the valence and sea quark actions are different, is inherently partially quenched and therefore violates unitarity. Unlike conventional partially quenched calculations, to restore unitarity, one must take the continuum limit in addition to tuning the valence and sea quark masses to be degenerate. This process is aided by the use of mixed-action chiral perturbation theory [38–43]. Given the situation, there is an ambiguity in the choice of the valence light-quark masses. One appealing choice is to tune the valence light quark masses such that the valence pion mass is degenerate with the Goldstone staggered pion mass. In the continuum limit, the \( N_f = 2 \) staggered action has a \( SU(8)_c \otimes SU(8)_s \otimes U(1)_V \) chiral symmetry due to the fourfold taste degeneracy of each flavor, and each pion has 15 degenerate partners. At finite lattice spacing this symmetry is broken and the taste multiplets are no longer degenerate, but have splittings that are \( \mathcal{O}(a^2) \) [21–23,26,44]. The propagators used in this work were tuned to give valence pions that match the Goldstone Kogut-Susskind pion. This is the only pion that becomes massless in the chiral limit at finite lattice spacing. As a result of this choice, the valence pions are as light as possible, while being tuned to one of the staggered pion masses, providing better convergence in the chiral perturbation theory needed to extrapolate the lattice results to the physical quark-mass point. This set of parameters, listed in Table I, was first used by LHPC [35,36] and utilized to compute the spectroscopy of hadrons composed of up, down and strange quarks [37]. A two-flavor chiral perturbation theory analysis on this action was recently performed for the pion mass and pion decay constant [45], finding good agreement with the lattice average of these quantities and their LECs.

B. Heavy-quark action

For the charm quark we use a relativistic heavy-quark action motivated by the Fermilab approach [46]. This action controls discretization errors of \( \mathcal{O}(am_0^3\alpha_s) \). Following the Symanzik improvement [47], an effective continuum action is constructed using operators that are invariant under discrete rotations, parity-reversal and charge-conjugation transformations, representing the long-distance limit of our lattice theory, including leading finite-\( a \) errors. Using only the Dirac operator and the gluon field tensor (and distinguishing between the time and space components of each), we enumerate seven operators with

```
<table>
<thead>
<tr>
<th>Ensemble</th>
<th>( \beta )</th>
<th>( am_u )</th>
<th>( am_d )</th>
<th>( am_c )</th>
<th>( N_{\text{cfgs}} )</th>
<th>( N_{\text{props}} )</th>
</tr>
</thead>
<tbody>
<tr>
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<td>0.007</td>
<td>0.050</td>
<td>0.0081</td>
<td>461</td>
<td>2766</td>
</tr>
<tr>
<td>M010</td>
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<td>0.010</td>
<td>0.050</td>
<td>0.0138</td>
<td>636</td>
<td>3816</td>
</tr>
<tr>
<td>M020</td>
<td>6.79</td>
<td>0.020</td>
<td>0.050</td>
<td>0.0313</td>
<td>480</td>
<td>1920</td>
</tr>
<tr>
<td>M030</td>
<td>6.81</td>
<td>0.030</td>
<td>0.050</td>
<td>0.0478</td>
<td>563</td>
<td>1689</td>
</tr>
</tbody>
</table>
```
dimension up to five. By applying the isospectral transformations \[48\], the redundant operators are identified and their coefficients are set to appropriate convenient values. The lattice action then takes the form

\[ S = S_0 + S_B + S_E, \tag{1} \]

with

\[ S_0 = \sum_x \vec{Q}(x) \left[ m_0 + \left( \gamma_0 \nabla_0 - \frac{a}{2} \Delta_0 \right) + \nu \sum_i \left( \gamma_i \nabla_i - \frac{a}{2} \Delta_i \right) \right] Q(x), \tag{2} \]

\[ S_B = -\frac{a}{2} c_B \sum_x \vec{Q}(x) \left( \sum_{i<j} \sigma_{ij} F_{ij} \right) Q(x), \tag{3} \]

\[ S_E = -\frac{a}{2} c_E \sum_x \vec{Q}(x) \left( \sum_{i<j} \sigma_{0i} F_{0i} \right) Q(x), \tag{4} \]

where the operator \( Q(x) \) annihilates a heavy-quark field, \( a \) is the lattice spacing, \( \nabla_0 \) and \( \nabla_i \) are first-order lattice derivatives in the time and space directions, \( \Delta_0 \) and \( \Delta_i \) are second-order lattice derivatives, and \( F_{\mu\nu} \) is the gauge field strength tensor. The spectrum of heavy-quark bound states can be determined accurately through \( [m \Lambda]^n \) for an arbitrary exponent \( n \) by using a lattice action containing \( m_0, \nu, c_B \) and \( c_E \), which are functions of \( amQ \).

The coefficients \( c_B \) and \( c_E \) are different due to the broken space-time interchange symmetry, which can be computed in perturbation theory by requiring elimination of the heavy-quark discretization errors at a given order in the strong coupling constant \( \alpha_s \). We use the tree-level tadpole-improved results obtained by using field transformation (as in Ref. \[48\]):

\[ c_B = \frac{\nu}{u_0}, \quad c_E = \frac{1}{2} (1 + \nu) \frac{1}{u_0^2}, \tag{5} \]

where \( u_0 \) is the tadpole factor

\[ u_0 = \left( \frac{1}{3} \sum_p \text{Tr}(U_p) \right)^{1/4}, \tag{6} \]

and \( U_p \) is the product of gauge links around the fundamental lattice plaquette \( p \). The remaining two parameters \( m_0 \) and \( \nu \) are determined nonperturbatively. The bare charm-quark mass \( m_0 \) is tuned so that the experimentally observed spin average of the \( J/\psi \) and \( \eta_c \) masses

\[ M_{\text{avg}} = \frac{1}{4} M_{\eta_c} + \frac{3}{4} M_{J/\psi} \tag{7} \]

is reproduced. For each ensemble, we calculate \( M_{\text{avg}} \) at two charm-quark masses (denoted \( m_1 = 0.2034 \) and \( m_2 = 0.2100 \)) and linearly extrapolate it to the experimental value to determine the parameter \( m_0 = m_c^{\text{phys}} \). The value of \( \nu \) must be tuned to restore the dispersion relation

\[ E_h^2 = m_h^2 + c^2 p^2 \]

such that \( c^2 = 1 \). To do this, we calculate the single-particle energy of \( \eta_c, J/\psi, D_s \) and \( D \) at the six lowest momenta (with unit of \( a^{-1} \): \( (2\pi/L)(0, 0, 0), (2\pi/L)(1, 0, 0), (2\pi/L)(1, 1, 0), (2\pi/L)(1, 1, 1), (2\pi/L) \times (2, 0, 0), (2\pi/L)(2, 1, 0) \)

For each ensemble, the energy levels are calculated at the two charm-quark masses \( (m_1 \) and \( m_2) \) and extrapolated to the physical charm-quark mass \( m_c^{\text{phys}} \). The values of \( c^2 \) are obtained by fitting the extrapolated energy levels to the dispersion relation. We tune \( \nu \) using the dispersion relation of \( \eta_c \). The dispersion relations for either the charmonium \( J/\psi \) or the charm-light mesons \( (D \) and \( D_s) \) are generally consistent with \( c^2 = 1 \) within \( 1\%–2\% \). Since the values of \( \nu \) and \( m_0 \) are coupled, one needs to iterate the tuning process in order to achieve a consistent pair of values. For the details of tuning the bare charm-quark mass \( m_0 \) and the value of \( \nu \), see Ref. \[49\].

### III. LÜSCHER’S FORMULA

Lüscher has shown that the scattering phase shift is related to the energy shift \( (\Delta E) \) in the total energy of two interacting hadrons in a finite box \[17,18\].

The center-of-mass momentum \( p \) can be obtained by the relation

\[ \Delta E = \sqrt{m_1^2 + p^2} + \sqrt{m_2^2 + p^2} - m_1 - m_2, \tag{8} \]

where \( m_1 \) and \( m_2 \) are the rest masses of the two hadrons.

To obtain \( p \cot \delta(p) \), where \( \delta(p) \) is the phase shift, we use the formula \[50\]:

\[ p \cot \delta(p) = \frac{1}{\pi L} S \left( \frac{p L}{2\pi} \right)^2, \tag{9} \]

where the \( S \) function is defined as

\[ S(x) = \sum_{|j| < \Lambda} \frac{1}{|j|^2 - x} - 4\pi \Lambda. \tag{10} \]

The sum is over all three-vectors of integers \( j \) such that \( |j| < \Lambda \), and the limit \( \Lambda \to \infty \) is implicit.

If the interaction range is much smaller than the lattice size, \( p \cot \delta(p) \) is given by

\[ p \cot \delta(p) = \frac{1}{a} + O(p^2), \tag{11} \]

where \( a \) is the scattering length (not to be confused with the lattice spacing which has the same notation and dimension). Note that we take the sign convention that a repulsive interaction has a negative scattering length. The higher-order terms in Eq. \( \text{(11)} \) can be ignored if the effective range of the interaction is much smaller than the length scale associated to the center-of-mass momentum \( p \). If we ignore the higher-order terms, the scattering length can be calculated by

\[ a = \pi L S^{-1} \left( \frac{p L}{2\pi} \right)^2. \tag{12} \]
IV. NUMERICAL RESULTS

In the following, we list all the channels we study. The interpolating operators for these two-particle states are

\[ O_{D_s/C25} = D_s^+ \pi^- + D_s^+ \pi^+ , \]
\[ O_{D_s/K} = D_s^+ K^- + D_s^+ K^+ , \]
\[ O_{I=0} = 3 \frac{s}{2} D_s/C25 , \]
\[ O_{I=1} = 1 \frac{s}{2} D_s/C22 , \]
\[ O_{I=3/2} = 1 \frac{s}{2} D_s/C25 , \]

where \( D_s^+ , D_s^+ , D_s^+ , K^- , K^+ \) and \( \pi^+ \) are the operators for one-particle states, the subscripts \( \pi , D , K \) and \( \bar{K} \) represent the isospin triplet \( (\pi^+ , \pi^0 , \pi^-) \) and doublets \( (D^+ , D^0) , (K^+ , K^0) \) and \( (\bar{K}^0 , K^-) \), respectively.

The total energy of two interacting hadrons \( (h_1 , h_2) \) is obtained from the four-point correlation function:

\[ G^{h_1 h_2}(t) = \langle O_{h_1 h_2}^{\dagger} O_{h_1 h_2}(0) \rangle . \]  (13)

To extract the energy shift \( \Delta E \), we define a ratio \( R^{h_1 h_2}(t) \):

\[ R^{h_1 h_2}(t) = \frac{G^{h_1 h_2}(t)}{G^{h_1 h_2}(0)} \exp(-\Delta E \cdot t) , \]  (14)

where \( G^{h_1}(t , 0) \) and \( G^{h_2}(t , 0) \) are two-point functions. \( \Delta E \) is obtained by fitting \( R^{h_1 h_2}(t) \) to a single exponential in the region where the effective mass exhibits a plateau.

For each channel, we calculate the ratio \( R^{h_1 h_2} \) at two different charm-quark masses and four different light-valence-quark masses. Figure 1 shows the effective energy shifts of each channel calculated from ensemble M007 at the bare charm-quark mass \( m_2 = 0.2100 \). The fitted energy shifts and the fitting ranges are indicated by the gray bars in these plots. The heights of the gray bars show the statistical errors.

**FIG. 1** (color online). Effective energy shift plots of the scattering channels \( D_s / \pi , D_s / K , D_s / \bar{K}(I = 0) , D_s / \bar{K}(I = 1) , D_s / \pi (I = 3/2) \). All plots are for ensemble M007. The gray bars show the fitted energy shifts and the fitting ranges. The heights of the gray bars show the statistical errors.
statistical errors. The $\chi^2$ per degree of freedom for these fits is presented in the plots. The fits of the energy shifts for other ensembles are similar.

The energy shifts are linearly extrapolated to the physical charm-quark mass on each ensemble.

V. CHIRAL EXTRAPOLATIONS OF THE SCATTERING LENGTHS

Because the simulations are performed at unphysical quark masses, chiral extrapolation is necessary in order to obtain the values of scattering lengths at the physical quark masses. There have been calculations based on chiral Lagrangians for these scattering lengths [51–54]. They were first calculated in Ref. [51] using a unitarized chiral approach. The basic observation is because of the coupled-channel effect and the large kaon mass, the interaction of some of the channels is so strong that a nonperturbatively, and calculated the scattering lengths up to one-loop order in chiral perturbation theory with \( \mathcal{O}(\Lambda) \) scale of dimensional regularization, and a change of \( \Lambda \) can be absorbed by a corresponding change of \( \hat{a}(\Lambda) \). The value \( \Lambda = 1 \text{ GeV} \) will be taken in the following. Promoting \( T(s) \), \( V(s) \) and \( G(s) \) to be matrix-valued quantities, it is easy to generalize Eq. (16) to coupled channels.

Using the \( \mathcal{O}(p^2) \) chiral Lagrangian constructed in Ref. [9], the scattering amplitudes are given by

\[
V(s, t, u) = \frac{1}{F^2} \left[ C_{\text{LO}} (s - u) - 4C_0 h_0 + 2C_1 h_1 
\right.

\[
- 2C_{24} H_{24}(s, t, u) + 2C_{35} H_{35}(s, t, u) \right]
\]

where \( F \) is the pion decay constant in the chiral limit, and the coefficients \( C_i \) can be found in Table II. Further,

\[
H_{24}(s, t, u) = h_2 p_2 \cdot p_4
\]

and

\[
H_{35}(s, t, u) = h_3 p_2 \cdot p_4 + h_5 (p_1 \cdot p_2 p_3 \cdot p_4 + p_1 \cdot p_4 p_2 \cdot p_3)
\]

with \( \sigma = \{[s - (m_1 + m_2)]^2\}^{1/2} \). The value \( \sigma \) is the scale of dimensional regularization, and a change of \( \lambda \) can be absorbed by a corresponding change of \( \hat{a}(\lambda) \). The value \( \Lambda = 1 \text{ GeV} \) will be taken in the following. Promoting \( T(s) \), \( V(s) \) and \( G(s) \) to be matrix-valued quantities, it is easy to generalize Eq. (16) to coupled channels.

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\right.

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\]

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V(s, t, u) = \frac{1}{F^2} \left[ C_{\text{LO}} (s - u) - 4C_0 h_0 + 2C_1 h_1 
\right.

\[
- 2C_{24} H_{24}(s, t, u) + 2C_{35} H_{35}(s, t, u) \right]
\]

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H_{35}(s, t, u) = h_3 p_2 \cdot p_4 + h_5 (p_1 \cdot p_2 p_3 \cdot p_4 + p_1 \cdot p_4 p_2 \cdot p_3)
\]
TABLE III. The values of scattering lengths for five channels in lattice units.

<table>
<thead>
<tr>
<th></th>
<th>$D\bar{K}(I = 1)$</th>
<th>$D\bar{K}(I = 0)$</th>
<th>$D\pi K$</th>
<th>$D\pi(I = 3/2)$</th>
<th>$D\pi\pi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>M007</td>
<td>-1.19(0.40)</td>
<td>5.34(1.45)</td>
<td>-1.58(0.14)</td>
<td>-1.16(0.30)</td>
<td>0.08(0.04)</td>
</tr>
<tr>
<td>M010</td>
<td>-1.89(0.12)</td>
<td>6.21(1.04)</td>
<td>-1.55(0.09)</td>
<td>-1.38(0.10)</td>
<td>0.08(0.03)</td>
</tr>
<tr>
<td>M020</td>
<td>-1.49(0.25)</td>
<td>4.43(1.33)</td>
<td>-1.40(0.20)</td>
<td>-1.08(0.30)</td>
<td>0.13(0.05)</td>
</tr>
<tr>
<td>M030</td>
<td>-1.59(0.13)</td>
<td>7.46(1.56)</td>
<td>-1.67(0.10)</td>
<td>-1.68(0.13)</td>
<td>0.32(0.05)</td>
</tr>
</tbody>
</table>

Note that the term $h_1\chi_+ = h_1(\chi_+ - \langle \chi_+ \rangle/3)$ in the Lagrangian in Refs. [57,58] has been replaced by $h_1\chi_+$, which amounts to a redefinition of $h_0$ (for the details of the Lagrangian and the definition of $\chi_+$, we refer to Refs. [59,51]). In this way, the $h_1$ term does not contain the $1/N_c$, with $N_c$ being the number of colors, suppressed part $\langle \chi_+ \rangle$ anymore. This was also done in Ref. [54].

In previous works [59,51], the large-$N_c$ suppressed LECs $h_0, h_4$ were dropped to reduce the number of parameters. However, when fitting to the lattice data at several unphysical quark masses, this is no longer necessary. In this work, we will keep all of the LECs at this order, and fit them to the lattice data. This strategy were also taken in Refs. [52–54], where the preliminary lattice results [14] were used. By definition, the LECs are independent of the pion mass. We further need to assume that the subtraction constant is the same for various channels, and neglect its pion mass dependence. In principle, this assumption is not necessary for a unitarization procedure matched to the full one-loop level of the perturbative calculation [57,58], which will be left for the future.

From the SU(3) mass splitting of the charmed mesons, the value of $h_1$ is fixed to be $h_1 = 0.42$. We still have six parameters, which are $\bar{a}, h_3, h_5, h_0, h_2$ and $h_4$. They are to be fitted to the lattice data. However, there is a high correlation between $h_3$ and $h_5$, as well as a similar correlation between $h_2$ and $h_4$. In the heavy quark limit, the $S$-wave projected amplitudes cannot distinguish the $h_{4(5)}$ terms from the $h_{2(3)}$ ones [59]. Hence, we may reduce the correlations largely by rewriting $H_{2a}(s, t, u)$ and $H_{35}(s, t, u)$ as

$$H_{2a}(s, t, u) = 2h_{2a}p_2 \cdot p_4 + h_4(p_1 \cdot p_2 p_3 \cdot p_4 + p_1 \cdot p_4 p_2 \cdot p_3 - 2\hat{M}_D^2 p_2 \cdot p_4),$$

and

$$H_{35}(s, t, u) = h_{35}p_2 \cdot p_4 + h_5(p_1 \cdot p_2 p_3 \cdot p_4 + p_1 \cdot p_4 p_2 \cdot p_3 - 2\hat{M}_D^2 p_2 \cdot p_4).$$

where $\hat{M}_D = (M_D^{phys} + M_D^{phys})/2$, the average of the physical masses of the $D$ and $D_s$ mesons, is introduced to match the dimensions. The new parameters $h_{2a}$ and $h_{35}$ are dimensionless, and their relations to the old ones are $h_{2a} = h_2 + h_4$ and $h_{35} = h_3 + 2h_5$, where $h' = h_M^2/\hat{M}_D^2$ and $h'' = h_M^2/\hat{M}_D^2$.

There are four different light quark masses in our data set, corresponding to the four ensembles (M007, M010, M020 and M030) with pion masses approximately 301 MeV, 364 MeV, 511 MeV and 617 MeV, respectively. There are in total 20 data points in the five channels. The values of the scattering lengths for all the channels are collected in Table III. In order to fit to the pion mass dependence of the results, we have to express the masses of the involved mesons in terms of the pion mass. They are the kaon, $D$ and $D_s$ mesons, and their masses in the four ensembles are listed in Table IV together with the corresponding pion masses and values of the lattice spacing. The masses of pion and kaon are taken from Ref. [37]. The masses of $D$ and $D_s$ mesons are from our calculations. The lattice spacing is set by $r_1$ in Ref. [60]. We will use

$$M_K = \frac{\hat{M}_K}{M_\pi},$$

$$M_D = \frac{\hat{M}_D}{(h_1 + 2h_0)},$$

$$M_{D_s} = \frac{\hat{M}_{D_s}}{2h_0}.$$

With $\hat{M}_K = 551.2$ MeV, $\hat{M}_D = 1942.9$ MeV, $\hat{M}_{D_s} = 2062.3$ MeV and $h_0 = 0.014$, the values at different pion masses shown in Table IV are well described. Note that,

TABLE IV. The masses of the pion, kaon, $D$ and $D_s$ mesons in lattice units. The values of the lattice spacing $a$ are also given in the last column [60].

<table>
<thead>
<tr>
<th></th>
<th>$M_\pi$</th>
<th>$M_K$</th>
<th>$M_D$</th>
<th>$M_{D_s}$</th>
<th>$a$ (fm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>M007</td>
<td>0.1842(7)</td>
<td>0.3682(5)</td>
<td>1.2081(13)</td>
<td>1.2637(10)</td>
<td>0.1207</td>
</tr>
<tr>
<td>M010</td>
<td>0.2238(5)</td>
<td>0.3791(5)</td>
<td>1.2083(11)</td>
<td>1.2635(10)</td>
<td>0.1214</td>
</tr>
<tr>
<td>M020</td>
<td>0.3113(4)</td>
<td>0.4058(4)</td>
<td>1.2226(13)</td>
<td>1.2614(12)</td>
<td>0.1202</td>
</tr>
<tr>
<td>M030</td>
<td>0.3752(5)</td>
<td>0.4311(5)</td>
<td>1.2320(11)</td>
<td>1.2599(12)</td>
<td>0.1200</td>
</tr>
</tbody>
</table>
with these values, both the kaon and charmed-meson masses at the physical pion mass are higher than their genuine physical values. For the kaon mass this is mainly due to the unphysical strange-quark mass in the lattice configurations. The strange-quark mass that gives the physical light-pseudoscalar-meson masses has been determined to be \(a m_s = 0.035(7)\) in Ref. [60], which is lighter than the value used in our calculations. The charmed-meson masses also suffer the discretization error arising both from light- and charm-quark actions. The effect of the discretization errors on the masses of charmed baryons has been investigated in Ref. [49]. It suggests that the discretization errors increase the singly charmed-baryon masses by around 70 MeV. It is reasonable to expect that the discretization errors increase the masses of \(D\) and \(D_s\) mesons. However, with the input masses of the kaon, \(D\) and \(D_s\) mesons all calculated from the lattices, the fit to the scattering lengths is self-consistent.

For a pion mass as high as 617 MeV, the kaon mass would be even higher, around 700 MeV. Such values are too large for a controlled chiral expansion. Therefore, we will only fit to the ensembles M007, M010 and M020. To minimize the contamination from a particular scale-setting method, we fit to the dimensionless product of the pion mass and the scattering length. The fit was performed using the FORTRAN package MINUIT [61]. The best fit has \(\chi^2/\text{d.o.f} = 1.06\), and the resulting parameters are collected in Table V, where the asymmetric 1\(\sigma\) uncertainties are calculated using the MINOS algorithm in MINUIT. A comparison of the best fit and the lattice data is shown in Fig. 2, where the solid curves correspond to the results of the best fit, and the bands reflect the uncertainties propagated from the lattice data. At the physical pion mass, the extrapolated scattering lengths for the five channels are presented in Table VI.

One can see that all the dimensionless parameters have a natural size, i.e., the absolute values of \(h_{24,35}\) and \(h'_{1,3,5}\) are of order unity. The value of \(h_0 = 0.014\) is much smaller than \(h_1 = 0.42\). This is consistent with the \(N_c\) counting because the \(h_0\) term is suppressed by \(1/N_c\) as compared to the \(h_1\) term. Furthermore, we also have the hierarchies \(|h'_{5}| < |h'_{3}|\) and \(|h_2| < |h_3|\) (recall that \(h_2 = h_{24} - h'_{4}\) and \(h_3 = h_{35} - 2h'_{5}\)). For both cases, the left-hand sides are suppressed by \(1/N_c\) as compared to the right-hand sides.

The uncertainties quoted so far were determined by the fit only. In addition one has to add the theory uncertainty from the method and order used for the chiral extrapolation. The latter may be quantified by observing that we performed an analysis to next-to-leading order in the chiral expansion with expansion parameter \(\chi = M_{\pi}/\Lambda_{\chi}\), where \(\Lambda_{\chi}\) denotes the typical hadronic scale of order 1 GeV. Thus we may estimate the uncertainty from the chiral expansion as \(\chi^2 \approx 0.09\), where we used the \(M_{\pi} = 300\) MeV, the lowest value of the lattice calculation. This may be  

<table>
<thead>
<tr>
<th>Fitting range</th>
<th>(\chi^2/\text{d.o.f} )</th>
<th>(\hat{a}(\lambda = 1\ \text{GeV}))</th>
<th>(h_{24})</th>
<th>(h'_{4})</th>
<th>(h_{35})</th>
<th>(h'_{5})</th>
</tr>
</thead>
<tbody>
<tr>
<td>M007–M020</td>
<td>1.06</td>
<td>(-1.88^{+0.07}_{-0.09})</td>
<td>(-0.10^{+0.05}_{-0.06})</td>
<td>(-0.32^{+0.35}_{-0.34})</td>
<td>(0.25 \pm 0.13)</td>
<td>(-1.88^{+0.63}_{-0.61})</td>
</tr>
</tbody>
</table>

FIG. 2 (color online). Fit to the data of the scattering lengths corresponding to ensembles M007–M020 in each channel. The superscript \((S, I)\) is the (strangeness, isospin) for each channel.
TABLE VI. The scattering lengths extrapolated to the physical light quark masses.

<table>
<thead>
<tr>
<th>Channels</th>
<th>$D\bar{K}(I = 1)$</th>
<th>$D\bar{K}(I = 0)$</th>
<th>$D_s\bar{K}$</th>
<th>$D\pi(I = 3/2)$</th>
<th>$D_s\pi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a$ (fm)</td>
<td>$-0.20(1)$</td>
<td>$0.84(15)$</td>
<td>$-0.18(1)$</td>
<td>$-0.100(2)$</td>
<td>$-0.002(1)$</td>
</tr>
</tbody>
</table>

TABLE VII. Scattering lengths of $D\pi(I = 1/2)$, $DK(I = 1)$ and $D_s\bar{K}$ at the physical pion mass predicted from the fit.

<table>
<thead>
<tr>
<th>Channels</th>
<th>$D\pi(I = 1/2)$</th>
<th>$DK(I = 0)$</th>
<th>$DK(I = 1)$</th>
<th>$D_s\bar{K}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a$ (fm)</td>
<td>$0.37^{+0.03}_{-0.02}$</td>
<td>$-0.84^{+0.17}_{-0.22}$</td>
<td>$0.07 \pm 0.03 + i(0.17^{+0.02}_{-0.01})$</td>
<td>$-0.09^{+0.06}_{-0.05} + i(0.44 \pm 0.05)$</td>
</tr>
</tbody>
</table>

regarded as a conservative estimate, for one might expect that the unitarization already includes the leading pion mass dependencies. There is no clear prescription to estimate the uncertainty from the method of unitarization employed. However, given the high quality achieved for the fit we assume this uncertainty to be small; clearly further studies are necessary.

When performing the fit, we have used the physical value for the pion decay constant $F = 92.21$ MeV [62]. The difference from the chiral limit value and hence its pion mass dependence is a higher-order effect, and is neglected here, although it might have some influence.

VI. IMPLICATIONS FOR OTHER CHANNELS

A. Scattering lengths

In this work we did not calculate the scattering lengths on the lattice for the channels whose Wick contractions involve disconnected diagrams due to the computational difficulties, as well as the additional lattice artifacts present in these channels due to the use of Kogut-Susskind sea quarks. However, once we have determined the LECs in the chiral Lagrangian, we can make predictions on the scattering lengths of these channels. The results for the scattering lengths of $D\pi(I = 1/2)$, $DK(I = 0)$, $DK(I = 1)$ and $D_s\bar{K}$ at the physical pion mass are presented in Table VII. For these predictions, we have required that the masses of the involved mesons at the physical pion mass coincide with their physical values, i.e., $\hat{M}_K = 485.9$ MeV, $\hat{M}_D = 1862.7$ MeV, $\hat{M}_{D_s} = 1968.2$ MeV are used. For $DK(I = 1)$, the imaginary part of the scattering length originates because it couples to $D_s\pi$ with a lower threshold. Similarly, $D_s\bar{K}$ couples to $D\pi$ and $D\eta$ so that the scattering length is complex, too. The result for the $D\pi(I = 1/2)$ channel is consistent with the indirect extraction from lattice calculations of the $D\pi$ scalar form factor $0.41 \pm 0.06$ fm [63]. At a pion mass of about 266 MeV, our prediction is $2.30^{+0.40}_{-0.60}$ fm, larger than the very recent full QCD calculation $(0.81 \pm 0.14)$ fm [15]. From Fig. 3, one sees that such a pion mass is close to the transition point where the scattering length changes sign due to the generation of a pole (for more discussions, see Ref. [51]). In such a region, the value of the scattering length changes quickly. For instance, decreasing the pion mass by 40 MeV, we would get a much smaller value $1.11^{+0.36}_{-0.17}$ fm.

The most interesting channel is the one with $(S,I) = (1,0)$, where the $D_s^*(2317)$ resides. This state was proposed to be a hadronic molecule with a dominant $DK$ component by several groups [64–68]. The attraction in this channel is so strong that a pole emerges in the

FIG. 3 (color online). Predicted pion mass dependence of the $D\pi(I = 1/2)$ and $DK(I = 0)$ scattering lengths using parameters from the five-parameter fit. The solid curves are calculated using the parameters from the best fit, and the bands reflect the uncertainties.
resummed amplitude. Within the range of 1σ uncertainties of the the parameters, there is always a pole on the real axis in the first Riemann sheet, which corresponds to a bound state. If we use the physical values for all the meson masses, the pole position is $2315^{+18}_{-28}$ MeV. The central value corresponds to the pole found using the best fit parameters. It is very close to the observed mass of the $D^{*}_{s0}(2317)$, $(2317.8 \pm 0.6)$ MeV [62], and it is found in the channel with the same quantum numbers as that state. Therefore, one is encouraged to identify the bound state pole with the $D^{*}_{s0}(2317)$.

As emphasized in, for instance, Refs. [69,70], if there is an $S$-wave shallow bound state, the scattering length is related to the binding energy, and to the wave function renormalization constant $Z$, with $(1 - Z)$ being the probability of finding the molecular component in the physical state (for $Z = 0$, the physical state is purely a bound state). The relation reads

$$a = -2 \frac{(1 - Z)}{2 - Z} \frac{1}{\sqrt{2} \mu \epsilon} (1 + \mathcal{O}(\sqrt{2} \mu \epsilon / \beta)),$$

where $\mu$ and $\epsilon$ are the reduced mass and binding energy, respectively. Corrections of the above equation come from neglecting the range of forces, $1/\beta$, which contains information of the $D_s \eta$ channel. Were the $D^{*}_{s0}(2317)$ a pure $DK$ bound state ($Z = 0$), the value of the $DK(I = 0)$ scattering length would be $a = -1.05$ fm, which coincides with the range in Table VII. From Eq. (20), the factor $Z$ is found to be in the range $[0.27, 0.34]$. This means that the main component of the pole, corresponding to the $D^{*}_{s0}(2317)$, is the $S$-wave $DK$ in the isoscalar channel.

B. Isospin breaking width of the $D^{*}_{s0}(2317)$

In the following, we will assume that the $D^{*}_{s0}(2317)$ corresponds to the pole generated in the $(S, I) = (1, 0)$ channel, and explore the implications of our lattice calculation on this state. We will fix the pole position to the mass of the $D^{*}_{s0}(2317)$, 2317.8 MeV [62], on the first Riemann sheet. We fit the lattice results of the scattering lengths with four parameters $h_{24}$, $h_{35}$, $h'_{4}$ and $h'_{5}$, and adjust the subtraction constant $\alpha(\lambda = 1$ GeV) to reproduce the mass of the $D^{*}_{s0}(2317)$. Again, we only fit to the ensembles M007, M010 and M020. The best fit gives $\chi^2$/d.o.f $= 0.97$, which is slightly smaller than the one with one more parameter in Sec. V. The parameter values together with the 1σ statistical uncertainties are given in Table VIII. The parameter values are similar to the ones obtained in the five-parameter fit, but with smaller uncertainties. All the dimensionless LECs are of natural size, and the $N_c$ hierarchies are the same as before.

### Table VIII. Results of fitting to the lattice data of the scattering lengths with four parameters. The subtraction constant is solved from fixing the pole in the $(S, I) = (1, 0)$ channel to 2317.8 MeV.

<table>
<thead>
<tr>
<th>Fitting range</th>
<th>$\chi^2$/d.o.f</th>
<th>$h_{24}$</th>
<th>$h'_{4}$</th>
<th>$h_{35}$</th>
<th>$h'_{5}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>M007–M020</td>
<td>0.97</td>
<td>$-0.10^{+0.05}_{-0.06}$</td>
<td>$-0.30^{+0.31}_{-0.28}$</td>
<td>$0.26^{+0.09}_{-0.10}$</td>
<td>$-1.94^{+0.46}_{-0.38}$</td>
</tr>
</tbody>
</table>

FIG. 4 (color online). Fit to the data corresponding to ensembles M007–M020 in each channel with four parameters. The subtraction constant is solved from fixing the pole in the $(S, I) = (1, 0)$ channel to 2317.8 MeV.
TABLE IX. The scattering lengths extrapolated to the physical light quark masses from the
four-parameter fit.

<table>
<thead>
<tr>
<th>Channels</th>
<th>$D\bar{K}(I = 1)$</th>
<th>$D\bar{K}(I = 0)$</th>
<th>$D_sK$</th>
<th>$D\pi(I = 3/2)$</th>
<th>$D_s\pi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a$ (fm)</td>
<td>$-0.21(1)$</td>
<td>$0.84(15)$</td>
<td>$-0.18(1)$</td>
<td>$-0.100(1)$</td>
<td>$-0.002(1)$</td>
</tr>
</tbody>
</table>

TABLE X. Scattering lengths of $D\pi(I = 1/2)$, $DK(I = 0)$, $DK(I = 1)$ and $D_sK$ at the
physical pion mass predicted from the four-parameter fit.

<table>
<thead>
<tr>
<th>Channels</th>
<th>$D\pi(I = 1/2)$</th>
<th>$DK(I = 0)$</th>
<th>$DK(I = 1)$</th>
<th>$D_sK$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a$ (fm)</td>
<td>$0.37 \pm 0.01$</td>
<td>$-0.86 \pm 0.03$</td>
<td>$0.04^{+0.05}<em>{-0.01} + i(0.16^{+0.02}</em>{-0.01})$</td>
<td>$-0.06^{+0.01}_{-0.05} + i(0.45 \pm 0.05)$</td>
</tr>
</tbody>
</table>

The fitted results are presented in Fig. 4. At the physical pion mass, the extrapolated values of the scattering lengths are listed in Table IX. The results are quite similar to the ones in the last section, yet with slightly smaller uncertainties.

With the newly fitted parameters, the scattering lengths for several other channels are predicted, and the results are listed in Table X. Again, the values are compatible with the ones in Table VII. One sees that the value for the $DK(I = 0)$ channel is close to the result of Eq. (19), $\pm 1.05$ fm, with $Z = 0$. The deviation from this value is partly due to the coupled-channel $D_s\eta$, and partly due to the energy dependence in the interaction. Using Eq. (19), the value of $Z$ is again in the range of $[0.27, 0.34]$. Both the stability of the fit and the small $Z$ indicates that the main component of the $D_{s0}^{*}(2317)$ is the isoscalar $DK$ molecule.

We show the predictions for the pion mass dependence of the scattering lengths for the $D\pi(I = 1/2)$ and $DK(I = 0)$ channels using parameters from this fit in Fig 5. The result for the $D\pi(I = 1/2)$ channel at the physical pion mass is still consistent with the indirect extraction, $(0.41 \pm 0.06)$ fm, in Ref. [63], and the result at $M_\pi = 266$ MeV, $2.09^{+0.31}_{-0.11}$ fm, is again larger than $(0.81 \pm 0.14)$ fm obtained in Ref. [15]. As before, in such a region, the value of the scattering length changes quickly. For instance, decreasing the pion mass to $220$ MeV, one would get a much smaller value $(0.98^{+0.06}_{-0.03})$ fm.

All the above calculations have assumed the same mass for the up and down quarks, and neglected the electromagnetic interaction. This is the isospin symmetric case. However, the $D_{s0}^{*}(2317)$ decays into the isovector final state $D_s\pi$. In order to calculate this isospin breaking decay width, one has to take into account both the up- and down-quark mass difference and virtual photons. This has been done in Ref. [9]. In Ref. [9], the $N_c$-suppressed operators, i.e., the $h_0$, $h_2$ and $h_4$ terms, have been dropped, and a somewhat arbitrarily chosen natural range $[-1, 1]$ was taken for $h_i$. The isospin breaking decay width was calculated to be $\Gamma(D_{s0}^{*}(2317) \to D_s\pi) = (180 \pm 110)$ keV [9].

With the values of all the $h_i$’s in Table VIII, the result is updated to be

$$\Gamma(D_{s0}^{*}(2317) \to D_s\pi) = (133 \pm 22)\text{ keV}. \quad (20)$$

We have used the isospin breaking quark mass ratio $(m_d - m_u)/(m_s - \tilde{m}) = 0.0299 \pm 0.0018$, where $\tilde{m} = (m_u + m_d)/2$, which is calculated using the lattice averages (up to end of 2011) of the light quark masses [71,72]. The error quoted in Eq. (20) comes from the uncertainties of the isospin breaking quark mass ratio, the $h_i$’s and the
chiral extrapolation—for this quantity we refer to the discussion at the end of Sec. V—all added in quadrature.

VII. SUMMARY AND DISCUSSION

The low-energy interaction between a light pseudoscalar meson and a charmed pseudoscalar meson was studied. We have calculated scattering lengths of five channels $D\bar{K}(I=0)$, $D\bar{K}(I=1)$, $D_sK$, $D\pi(I=3/2)$ and $D_s\pi$ with four ensembles. Among these channels, the interaction of $D\bar{K}(I=0)$ is attractive, and that of the others is repulsive. The interaction of $D_s\pi$ is very weak, which is expected. The $D_s\pi$ and $D\bar{K}(I=1)$ channels are mixed since they have the same quantum numbers. To perform a more reliable analysis of these two channels, we need to construct the correlation matrix and use the variational method to extract the energies of the two channels. The chiral extrapolation was performed using SU(3) unitarized chiral perturbation theory, and the LECs $h_i$’s in the chiral Lagrangian were determined from a fit to the lattice results. With the same set of LECs and the masses of the involved mesons set to their physical values, we made predictions on other channels including $D\bar{K}(I=0)$, $D\bar{K}(I=1)$, $D\pi(I=1/2)$ and $D_s\bar{K}$. In particular, we found that the attractive interaction in the $D\bar{K}(I=0)$ channel is strong enough so that a pole is generated in the unitarized scattering amplitude. Within 1σ uncertainties of the parameters, the pole is at $2315^{+18}_{-28}$ MeV, and it is always below the $DK$ threshold. From calculating the wave function normalization constant, it is found that this pole is mainly an $S$-wave $DK$ bound state. By further fixing the pole to the observed mass of $D_s^0(2317)$, we revisited the isospin breaking decay width of the $D_s^0(2317)\to D_s\pi$. The result $(133\pm22)$ keV updates the old result $(180\pm110)$ keV obtained in Ref. [9]. It is nice to see that the uncertainty of the width shrinks a lot. We want to stress that the width is much larger than the isospin breaking width of a $c\bar{s}$ meson, which is of the order of 10 keV.

It is possible to further constrain the values of $h_i$’s once simulations in other channels are done. Although a precise calculation of the other channels requires disconnected diagrams, one may obtain valuable information from the connected part only. The connected and disconnected parts can be calculated separately using partially quenched chiral perturbation theory (for reviews, see Refs. [73,74]); then a fit to the lattice calculation can be performed.

This point has already been stressed, for instance, in Ref. [75] for the hadronic vacuum polarization and in Ref. [76] for the scalar form factor of the pion. In our chiral extrapolation, the resummed chiral amplitude is of $O(p^2)$. At this order, there is no counterterm to absorb the divergence of the loop function $G(s)$, because loops only start from $O(p^3)$. As a result, we had to regularize the divergent loop by a subtraction constant. The pion mass dependence of the latter was neglected. Were a full one-loop calculation available, the chiral amplitudes can be renormalized at one-loop order, and the representation of the pion mass dependence would be improved. However, more unknown LECs will be introduced in this way, and it is difficult to perform a fit with all of them to the present data. As mentioned above, more data can come from calculating the other channels, which is useful even if the disconnected contribution is neglected. Such a study with an improved chiral extrapolation is relegated to the future.

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