Evidence for a doubly charm tetraquark pole in $DD^*$ scattering on the lattice

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The doubly charm tetraquark with flavor $cc\bar{u}\bar{d}$ and isospin $I = 0$ is investigated by calculating the $DD^*$ scattering amplitude with lattice QCD. The simulation is done on CLS ensembles with dynamical $u/d, s$ quarks and $m_s \simeq 280$ MeV for two charm quark masses, one slightly larger and one slightly lower than the physical value. The scattering amplitudes for partial waves $l = 0, 1$ are extracted near-threshold via the Lüscher’s method by considering systems with total momenta $PL/(2\pi) = 0, 1, \sqrt{2}, 2$ on two spatial volumes. A virtual bound state pole in the $DD^*$ scattering amplitude with $l = 0$ is found $9.9^{+2.4}_{-1.7}$ MeV below $DD^*$ threshold for the charm quark mass closer to the physical value. This pole is likely related to the doubly charm tetraquark discovered by LHCb.

Introduction: The LHCb collaboration recently discovered a doubly charmed tetraquark $T_{cc}$ with flavor $cc\bar{u}\bar{d}$ just $0.36(4)$ MeV below $D^0 D^{*+}$ threshold $^{[1,2]}$. Its flavor is based on the decay channel $D^0 D^{*+}\pi^+$ and it has isospin $I = 0$ since no state was found in the decay $D^0 D^{*+}\pi^+$. The total spin and parity $J^P$ have not been determined from experiment.

Several phenomenological models predicted a doubly charm tetraquark $cc\bar{u}\bar{d}$ with $I = 0$ and $J^P = 1^+$ within an energy range $\pm 100$ MeV around the $DD^*$ threshold, c.f. Refs. $^{[3,11]}$. Many of these models have a possibility to identify a bound state but not a resonance. One of the more sophisticated quark model calculations predicted the bound state $1.6 \pm 1.0$ MeV below $DD^*$ threshold and concluded that the molecular Fock component dominates over the diquark antidiquark component $^{[10]}$. Within a molecular picture, a light vector meson exchange is argued to induce attraction $^{[12,14]}$, whereas one-pion exchange induces slight repulsion $^{[14]}$. The binding energy of a bound state in the $QQ\bar{u}\bar{d}$ system is found to decrease with decreasing heavy quark mass $m_Q$ and increasing light quark mass $m_{u,d}$. $^{[8,10,17,19,20,22]}$. Thus the doubly bottom tetraquarks $bb\bar{u}\bar{d}$ and $bb\bar{s}\bar{s}$ with $J^P = 1^+$ are strongly bound and stable below $BB^*$ threshold according to variety of theoretical approaches $^{[8,11,15,17,19,20,22]}$, whereas $cc\bar{u}\bar{d}$ is expected on the verge of binding and requires a careful theoretical study within QCD.

In order to confirm the existence of a doubly charmed tetraquark from first-principles, one has to establish a pole singularity in the corresponding scattering amplitude $t(E_{cm})$. This is particularly important in finite-volume formulation of hadron-hadron scattering, such as lattice QCD, since this state does not lie well below the threshold but is expected near threshold. The scattering amplitude has not been determined using lattice simulations yet. The lattice study in Ref. $^{[15]}$ extracted the finite-volume energy of the ground state using meson-meson and diquark-antidiquark interpolators for a wide range of $m_\pi \geq 260$ MeV and three lattice spacings. The continuum and chiral extrapolations lead to an energy level $- 23 \pm 11$ MeV relative to the $DD^*$ threshold. This indicates the presence of interactions between $D$ and $D^*$, but does not prove the existence of a pole and a related state. The finite-volume energies have been extracted by the Hadron Spectrum Collaboration and the ground state energy was found to be consistent with the $DD^*$ threshold $^{[24]}$.

This letter investigates if a state with flavor $cc\bar{u}\bar{d}$, $I = 0$, and $J^P = 1^+$ exists in the vicinity of $DD^*$ threshold. For this purpose, $DD^*$ scattering amplitude $t(E_{cm})$ near threshold is extracted within lattice QCD for the first time. The scattering amplitude is determined from finite-volume energies via the Lüscher’s method $^{[25]}$. $D^*$ does not decay strongly to $D\pi$ at the simulated $m_\pi \simeq 280$ MeV and the analyzed energy region is below the $DD\pi$ and $D^*D^*$ thresholds, therefore we consider one-channel $DD^*$ scattering. We demonstrate that the scattering amplitude $t(E_{cm})$ indeed has a pole at $E^*_{cm}$ slightly below threshold and we extract the energy of $T_{cc}$ as $\text{Re}(E^p_{cm})$.

We first present the calculation of energy levels on the lattice. These then provide the scattering amplitude and location of the pole related to $T_{cc}$, which is finally compared to the LHCb discovery.

Ensembles and single-hadron masses: The simulation is done on two ensembles with $u/d, s$ dynamical quarks provided by the Coordinated Lattice Simulations (CLS) consortium $^{[26,27]}$. The lattice spacing is $a = 0.08636(98)(40)$ fm, $m_\pi$ and $m_d$ are degenerate and heavier than in Nature, corresponding to $m_\pi = 280(3)$ MeV. We utilize 255 configurations on spatial volume $N_{s^3} = 24^3$ and 492 configurations on $32^3$ with periodic boundary conditions in space. The scattering amplitude is extracted for two values of the charm quark mass, one
slightly heavier than physical and one slightly lighter \cite{29}. The masses of the relevant hadrons $D$ and $D^*$ are presented in Table I. The heavier charm quark mass is closer to the physical value and provides our main result.

**Interpolators and finite-volume energies:** In the non-interacting limit, the $DD^*$ system has discrete energies on a lattice of size $L = N_L a$

$$E_n^\ell = E_{D^*} (\vec{p}_I) + E_{D^*} (\vec{p}_J), \quad \vec{p}_I = \vec{n}_I \frac{2\pi}{L}, \quad \vec{n}_I \in N_L^3$$

with $E_{\text{con}}^\ell (\vec{p}_I) = (m^2_H + \vec{p}^2)^{1/2}$ in the continuum limit. The relevant non-interacting energies are shown by lines in Fig. 1.

The finite-volume energy levels in the interacting theory are determined from the two point correlation matrices $C_{ij} (t) = \langle O_i (t_{\text{src}} + t) O_j (t_{\text{src}}) \rangle$, where $O_i$ refers to operators that interpolate to the desired quantum numbers. In this study, we compute $C_{ij} (t)$ for the $cc\bar{u}\bar{d}$ system in inertial frames with total momenta $|\vec{P}| L / (2\pi) = 0, 1, \sqrt{2}, 2$ in different finite-volume irreducible representations (irreps) in Table I. These constrain the near-threshold $DD^*$ scattering amplitudes, of which partial wave $t = 0$ is expected to dominate. We utilize only meson-meson interpolators, where each meson is projected to a definite momentum,

$$O^{DD^*} = \sum_{k,j} A_{kj} D (\vec{p}_{1k}, \vec{p}_{2k}) + \vec{P}$$

with two choices $\Gamma_j = (\gamma_5, \gamma_j, (\gamma_5 \gamma_t, \gamma_j \gamma_t)$ throughout. The linear combinations of momenta and $D^*$-meson polarizations are chosen such that the operators transform according to the finite-volume irreps \cite{39}. For example, the explicit expressions for $DD^*$ interpolators in the $T_1$ irrep are

$$O_{l=0} = D (\vec{0}), \quad O_{l=0} = \sum_{\pm \vec{e}_{x,y,z}} D (\vec{e}_t) D^*_t (-\vec{e}_t)$$

$$O_{l=2} = \sum_{\pm \vec{e}_{x,y}} D (\vec{e}_t) D^*_t (-\vec{e}_t) - 2 \sum_{\pm \vec{e}_z} D (\vec{e}_t) D^*_t (-\vec{e}_t).$$

Other interpolators and partial waves $l$ that contribute are listed in Table I. All quark fields are smeared according to the ‘Distillation’ method \cite{29, 31} with 60(90) Laplacian eigenvectors for $N_L = 24(32)$. The correlation matrices are averaged over all spin and momentum polarizations and over several source timeslices $t_{\text{src}}$.

The diquark-antidiquark interpolators $[cc][\bar{d}\bar{u}]$ are not considered in this work. This is justified as it was observed in an earlier lattice calculation that such operators have negligible effects on the low-lying finite-volume energies in $cc\bar{u}\bar{d}$ system \cite{34}. Indications from phenomenological studies (c.f. Ref. [10]) on the dominance of molecular $DD^*$ Fock components also suggest that $DD^*$ interpolators are sufficient to compute the finite-volume energies faithfully. Furthermore, the application of two operators $D_{cc} D_{\bar{d}\bar{u}}$ and $D_{\gamma\gamma} D_{\gamma\gamma}$ for each momentum combination is expected to provide enough variety to extract the energy levels reliably.

The finite-volume energy levels $E_{\text{lat}}$ are extracted from single-exponential fits to the eigenvalue correlators $\lambda^{(n)} (t) \propto e^{E_{\text{lat}} t}$ of the generalized eigenvalue problem $C(t)^{\ell} (t) = \lambda^{(n)} (t) C(t) e^{(n) t}$ with $t_0 = 4 \sqrt{2}$. In order to mitigate small deviations of single-hadron energies $E_{\text{lat}}^{\ell}$ from $E_{\text{con}}^{\ell}$ due to discretization effects, we take $E_n = E_{\text{lat}} + E_{\text{con}}^{\ell} (\vec{p}_I) + E_{\text{con}}^{\ell} (\vec{p}_J) - E_{\text{lat}} D^* (\vec{p}_I) - E_{\text{lat}} D^* (\vec{p}_J)$ as the final energies for the scattering analysis, as argued and utilized for charmonium spectroscopy on the same ensembles in Refs. [29, 33].

The resulting finite-volume energies in all the irreps considered are presented in Fig. 1 for the heavier charm quark mass. The figure displays the corresponding energies $E_{\text{cm}} = (E^2 - \vec{P}^2)^{1/2}$ in the center-of-momentum frame in units of energy of the $DD^*$ threshold. The large circles and squares refer to the energy levels extracted from the lattice simulation. The non-interacting energies are shown by lines. The energy levels have nonzero energy shifts with respect to the noninteracting $DD^*$ energies Eq. (1) indicating nontrivial interactions. These energy shifts render information on the $DD^*$ scattering amplitudes. We find similar observations also for energies at our lighter charm quark mass \cite{39}.

**Scattering analysis:** The scattering amplitude $t = E^{2i\delta} = 1 + i \frac{4p}{E_{\text{cm}} - t}$ depends on energy, the partial wave $l$ and $J = |s - l|, ... , |s + l|$, where $s = 1$ for $DD^*$ system. We approximate their energy dependence near threshold with two terms of the effective range expansion in $p^2$ \cite{27}

$$t^{(J)} = \frac{E_{\text{cm}}}{2} \frac{1}{p_c \cot \delta^{(J)} - i p}, \quad p^{2J+1} \cot \delta^{(J)} = \frac{1}{a^{(J)}} + \frac{r^{(J)}}{2} - p^2,$$

where $p = |\vec{p}|$ is the spatial-momentum of $D$ and $D^*$ in the center-of-momentum frame. Each finite-volume energy level $E_{\text{cm}}$ is related to the $t^{(J)} (E_{\text{cm}})$ via Lüscher’s relation \cite{25} and its generalizations, e.g. \cite{34}. In order to constrain the energy dependence of $t$, the parameters of the effective range expansion are optimized such that Lüscher’s relation is simultaneously satisfied for all the energy levels considered in the analysis. For the $l = 0$ partial wave, which dominates near threshold, we find

$$p \cot \delta^{(J=1)} = \frac{1}{a^{(1)}} + \frac{1}{2} \frac{r^{(1)}}{p^2}$$

$$m_c^{(h)} : \quad a^{(1)} = 1.04(29) \, \text{fm}, \quad r^{(1)} = 0.96(0.18) \, \text{fm}. $$

This fit is shown by the red line in Fig. 2.

\footnote{This relation omits mixing of partial waves for reasons discussed later, while the more general relation is provided in Ref. [29].}
TABLE I. Total momenta $\vec{P}$, spatial lattice symmetry group ($LG$), irreducible representations ($\Lambda^P$) and interpolators considered for the system $cc\bar{u}\bar{d}$, together with total spin-parity $J^P$ and partial-wave $l$ of $DD^*$ scattering that contributes to each irrep (only $J,l \leq 2$ are listed). The interpolators are denoted by [2] when two linearly independent combinations of momenta and polarizations are employed, e.g. $O_{l=0,2}$ for $D(1)D^*(1)$ in $T_1^+$ (Eq. (5)).

| $\vec{P}$ | $LG$ | $\Lambda^P$ | $J^P$ | $l$ | interpolators: $M_1(\vec{p}_1^2)M_2(\vec{p}_2^2)$ |
|----------|------|--------------|------|----|-----------------------------------------------|
| (0, 0, 0) | $O_h$ | $T_1^+$      | 1$^+$ | 0, 2 | $D(0)D^*(0)$, $D(1)D^*(1)$ [2], $D^*(0)D^*(0)$ $D(1)D^*(1)$ |
| (0, 0, 0) | $O_h$ | $A_1^+$      | 0$^-$ | 1   | $D(1)D^*(1)$ $D(1)D^*(0)$ $D(0)D^*(1)$ $D(1)D^*(1)$ |
| (0, 0, 1)$^{3\pi/2}$ | Dic$_4$ | $A_2$ | 0$^-$, 1$^+$, 2$^-$ | 0, 1, 2 | $D(0)D^*(1)$ $D(1)D^*(1)$ $D(0)D^*(2)$ $D(1)D^*(1)$ [2], $D(2)D^*(1)$ |
| (1, 1, 0)$^{3\pi/2}$ | Dic$_2$ | $A_2$ | 0$^-$, 1$^+$, 2$^-$, 2$^+$ | 0, 1, 2 | $D(0)D^*(2)$ $D(1)D^*(1)$ [2], $D(2)D^*(1)$ |
| (0, 0, 2)$^{3\pi/2}$ | Dic$_4$ | $A_2$ | 0$^-$, 1$^+$, 2$^-$ | 0, 1, 2 | $D(1)D^*(1)$ |

FIG. 1. The center-of-momentum energy $E_{cm} = (E^2 - \vec{P}^2)^{1/2}$ of the $cc\bar{u}\bar{d}$ system normalized by $E_{DD^*} = m_D + m_{D^*}$, for the heavier charm quark mass in various finite-volume irreps. The lattice energy levels are shown by large circles and squares: the extraction of $DD^*$ scattering amplitude with $l = 0, 1$ employs the blue and green circles. The non-interacting $DD^*$ energies (only $J,l \leq 2$ are listed). The interpolators are denoted by [2] when two linearly independent combinations of momenta and polarizations are employed, e.g. $O_{l=0,2}$ for $D(1)D^*(1)$ in $T_1^+$ (Eq. (5)).

This result is robust to various fits we have performed. $J^P = 1^+$ is allowed for the $DD^*$ system with spin one in partial waves $l = 0$ and $l = 2$, which could lead to a partial wave mixing. We find that $t_2^{(1)}$ is consistent with zero, since the energy levels with dominant overlaps to $O_{l=2}$ [3] has energies consistent with the non-interacting energy [1]. Hence we assume $t_2^{(1)} = 0$ and that there is negligible mixing of $l=2$ with $l=0$ in $J=1$ [30]. The energies colored by blue and green from Fig. 1 are utilized to constrain the energy dependence of $t_0^{(1)}$ in Eq. (5) and $t_1^{(0)}$. We employ a combination of procedures outlined in Refs. [35, 36] in making our fits [30].

The fit has $\chi^2/\text{dof} = 3.7/5$ and renders the parameters in Eq. (5) for $l = 0$ scattering and $(a_1^{(0)}) = 0.076_{-0.008}^{+0.008}$ fm$^3$, $r_1^{(0)} = 6.9(2.1)$ fm$^{-1}$ for $l = 1$ scattering. The fit results for $t_1^{(0)}$ render poles significantly below threshold at energies that are unconstrained by the energy levels used in the analysis, and therefore we do not ascribe them any physical significance. The analytically predicted energies using $t_0^{(1)}$ in Eq. (5) and $t_1^{(0)}$ fits, and choosing $t_1^{(3)} = 0$, are given by the orange stars in Fig. 1 and agree well with the observed energies in all five irreducible representations, having $\chi^2/\text{dof} = 23/14$. An alternative fit, employing only partial wave $l = 0$ and only five low-lying...
energies from $T_1^+$ and $A_2(P = 1)$ irreps shown by blue and green circles in Fig. [2] leads to results consistent with those in Eq. [3].

We find a virtual bound state pole in $DD^*$ scattering amplitude $t_{(J=1)}^{(l=0)}$ at energy $E_{cm}^p = (m_D^2 - |p_B|^2)^{1/2} + (m_D^2 - |p_B|^2)^{1/2}$. It corresponds to the binding momentum indicated by the magenta octagon in Fig. [2]. We therefore find an evidence for the doubly charmed tetraquark as a virtual bound state

$$m_c^{(h)}: \delta m_{T_{cc}} = E_{cm}^p - m_D - m_{D^*} = -9.9^{+3.6}_{-7.1} \text{ MeV (6)}$$

situates slightly below $DD^*$ threshold, close to the mass of the doubly charmed tetraquark $T_{cc}$ discovered by LHCb [1, 2]. The state found on the lattice is strongly stable and the pole lies on the real axes since $D^* \to D\pi$ is not kinematically allowed for $m_Q \simeq 280$ MeV. The $T_{cc}$ discovered by LHCb decays to $D^0\bar{D}^0\pi^+$ and the pole is slightly imaginary, as shown in Fig. [3]. The $T_{cc}$ found in experiment would be a bound state in the limit of stable $D^*$ since the related scattering length $a_0^{(1)}$ is negative [2].

We expect that the virtual bound state pole found in our lattice simulation at unphysical $u/d$ masses is related to the $T_{cc}$ discovered by LHCb. The would-be LHCb bound state is expected to become a virtual bound state with increasing $m_{u/d}$. This is sketched in Fig. [4] for a tetraquark with a significant molecular $DD^*$ component attracted by the Yukawa-like potential $V(r) \propto e^{-M}\pi/r$, where the mass of the exchanged light hadron $M$ increases with increasing $m_{u/d}$.

A near-threshold virtual bound state pole is also observed for the lighter charm quark mass with a slightly larger $|\delta m_{T_{cc}}|$, as listed in Table [1]. This increase in the binding energy is also consistent with the dependence of the pole position on $m_Q$ sketched for the molecular component in Fig. [4]. This arises within quantum mechanics via the reduced $DD^*$ mass for purely attractive potential $V(r)$ that is assumed to be flavor blind. The influence of the virtual bound state pole on the scattering above threshold is diminished as the pole moves further below threshold with decreasing $m_c$.

**Conclusions:** We have performed the simulation of $DD^*$ scattering in lattice QCD at $m_Q \simeq 280$ MeV. Unlike other existing lattice investigations in this regard, we extracted the near-threshold scattering amplitudes in the flavor channel $cc\bar{u}\bar{d}$ with isospin $I = 0$. Scattering amplitudes for partial waves $l = 0, 1$ are determined via the Lüscher’s method, and a virtual bound state pole is found for the partial wave $l = 0$. The doubly charm tetraquark with $J^P = 1^+$ features as a virtual bound state with a binding energy of $9.9^{+3.6}_{-7.1} \text{ MeV}$ in our simulation with charm quark mass slightly larger than physical. We also observe that the size of the binding energy for this virtual bound state increases with decreasing charm quark mass.

A feature in the scattering amplitude. A bound state corresponds to a pole below threshold with binding momentum $p = i|p_B|$, whereas a virtual bound state has $p = -i|p_B|$ - it is not an asymptotic state and represents a feature in the scattering.

$\delta m = E_{cm}^p - E_{th}$ increasing $m_{u/d}$ or decreasing $m_c$. 

**The pole in the $DD^*$ scattering amplitude and $T_{cc}$:** The existence a hadron state and its mass are inferred from the pole in the scattering amplitude. A bound state corresponds to a pole below threshold with binding momentum $p = i|p_B|$, whereas a virtual bound state has $p = -i|p_B|$ - it is not an asymptotic state and represents a feature in the scattering.

3 Or else, the lattice results for the binding energy at various heavy quark masses can be used to examine how good is the heavy flavor symmetry in line with Ref. [55].
TABLE II. Lattice results for the binding energy $\delta m_{cc}$ and the effective range parameters in Eq. (4) at heavier ($m_{c}^{(h)}$) and lighter ($m_{c}^{(l)}$) charm quark masses, compared to experiment. $m_{c}^{(h)}$ is closer to the physical value according to the spin averaged charmonium mass $M_{cc} \equiv \frac{1}{2}(m_{c} + 3m_{J/\psi})$. The real part of experimental $a_{0}^{(1)}$ is provided. The binding energy $\delta m_{cc} \equiv \text{Re}(E_{cm}^{p}) - m_{D^{*}} - m_{D^{++}}$ is obtained from the energy $E_{cm}^{p}$, where the scattering amplitude has a pole.

| m_{D} [MeV] | m_{D^{*}} [MeV] | M_{cc} [MeV] | a_{0}^{(1)} [fm] | r_{cc}^{(J=1)} [fm] | $\delta m_{cc}$ [MeV] | T_{cc} |
|--------------|-----------------|---------------|----------------|-----------------|-------------------|-------|
| lat. ($m_{c} \simeq 280$ MeV, $m_{c}^{(h)}$) | 1927(1) | 2049(2) | 3103(3) | 1.04(29) | 0.96(0.18$^{+0.20}_{-0.20}$) | $-9.9^{+3.6}_{-7.2}$ | virtual bound st. |
| lat. ($m_{c} \simeq 280$ MeV, $m_{c}^{(l)}$) | 1762(1) | 1898(2) | 2820(3) | 0.86(0.22) | 0.92(0.17$^{+0.19}_{-0.19}$) | $-15.0^{+49.5}_{-9.3}$ | virtual bound st. |
| exp. | 1864.85(5) | 2010.26(5) | 3068.6(1) | $-7.15(51)$ | $-11.9(16.9,0)$ | $-0.36(4)$ | bound st. |

Outlook: Future investigations, including diquark-antidiquark interpolators and at smaller lattice spacings, are highly desired to reaffirm our findings and inferences. The simulations at smaller $m_{u/d}$ are also required to establish whether the pole will approach the $D^{*}$ threshold. The simulations at physical $m_{u/d}$ will be challenging due to the strong decays $D^{*} \to D\pi$ and $T_{cc} \to DD\pi$.

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See the supplemental material. This contains details of the operators utilized, the fitting procedure, the results from amplitude fits and discussion on heavy quark mass.
dependence of the near-threshold state.

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Supplemental material

This supplemental material provides further information on our study of the doubly charm tetraquark channel. We present the interpolators relevant for the scattering of a pseudoscalar particle and a vector particle and the details on how the corresponding scattering amplitudes are extracted. We also discuss the dependence of the pole position based on simple quantum mechanical arguments.

I. INTERPOLATORS

This section presents the explicit expressions for two-meson interpolators that transform according to the irreducible representations \( \Lambda \) in Table I of the main article. They are relevant for the scattering of a pseudoscalar meson \( P \) and a vector meson \( V \), so they are valuable for \( DD^* \) scattering simulated in this work and also for many interesting channels like \( BB^*, \pi J/\psi, KD^* \) etc. Each meson is projected to a definite momentum, which is given in units of \( 2\pi/L \) in parenthesis. The linear combinations of momenta and vector-meson polarizations are obtained with the partial-wave method for total momentum \( \vec{P} = \vec{0} \) \cite{39}. For \( \vec{P} \neq \vec{0} \) we consider only the one-dimensional irreducible representations and the operators are obtained with the projection method as \( O = \sum_{R \in LC} \chi^\Lambda(R) \, R \, P(\vec{p}_1) V_2(\vec{p}_2) \, R^{-1} \), where \( \chi^\Lambda(R) \) is the character. The operators indicated by \( \hat{O} \) were analyzed in the present simulation, while operators indicated by \( O' \) were not implemented and may be valuable for future studies:

\[
\begin{align*}
T_j^+ & : \vec{P} = \{0,0,0\}, \text{ row } z \\
O^{\text{a}=0} & = P(\{0,0,0\}) V_z(\{0,0,0\}) \\
O^{\text{a}=0} & = P(\{1,0,0\}) V_z(-1,0,0) + P(\{-1,0,0\}) V_z(1,0,0) \\
& + P(0,1,0) V_z(-1,0,0) + P(0,-1,0) V_z(0,1,0) \\
& + P(0,0,1) V_z(0,0,1) + P(0,0,-1) V_z(0,0,1) \\
O^{\text{a}=2} & = P(\{1,0,0\}) V_z(-1,0,0) + P(\{-1,0,0\}) V_z(1,0,0) \\
& + P(0,1,0) V_z(-1,0,0) + P(0,-1,0) V_z(0,1,0) \\
& - 2P(0,0,1) V_z(0,0,1) + P(0,0,-1) V_z(0,0,1) \\
O^{\text{a}=0} & = V_{1z}[0,0,0]V_{2z}[0,0,0] - V_{1z}[0,0,0]V_{2z}[0,0,0]
\end{align*}
\]

\[
\begin{align*}
A_j^+ & : \vec{P} = \{0,0,0\} \\
O & = P(\{1,0,0\}) V_z(-1,0,0) - P(\{-1,0,0\}) V_z(1,0,0) \\
& + P(0,1,0) V_\phi(-1,0,0) - P(0,-1,0) V_\phi(0,1,0) \\
& + P(0,0,1) V_z(-1,0,0) - P(0,0,-1) V_z(0,0,1) \\
A_j & : \vec{P} = \{0,0,1\} \\
O & = P(\{0,0,0\}) V_z(\{0,0,1\}) \\
O' & = P(\{1,0,1\}) V_z(\{-1,0,0\}) - P(\{-1,0,1\}) V_z(\{1,0,0\}) \\
& + P(0,1,1) V_\phi(-1,0,0) - P(0,-1,1) V_\phi(0,1,0) \\
O' & = P(\{1,0,1\}) V_z(-1,0,1) - P(\{-1,0,1\}) V_z(\{1,0,1\}) \\
& + P(0,1,1) V_\phi(-1,0,1) - P(0,-1,1) V_\phi(0,1,1) \\
O' & = P(\{1,0,0\}) V_z(-1,0,1) + P(\{-1,0,0\}) V_z(\{1,0,1\}) \\
& + P(0,1,0) V_z(-1,0,1) + P(0,-1,0) V_z(0,1,1)
\end{align*}
\]

The number of pseudoscalar-vector eigen-states is equal to the number of interpolators in the non-interacting limit. This renders degenerate eigenstates in non-interacting limit that are indicated by \( [2] \) in Fig. 1 of the main article. This is responsible for nearly degenerate states in interacting theory - we observe all the expected nearly degenerate states in our finite volume energy levels. The current study also employs the \( D^*D^* \) interpolator for the \( T_1^+ \) irrep and considers the levels below \( D^*D^* \) threshold in the scattering analysis.

II. DETAILS OF SCATTERING ANALYSIS

In this section, we discuss the details of our procedure for extracting the scattering amplitude \( t \) in Eq. (3) from the finite-volume energies and present a summary of various fits we have performed. The best fit values of parameters in the effective range expansion describing the energy dependence of \( t \) are determined by minimizing a \( \chi^2 \) function defined as

\[
\chi^2(\{a\}) = \sum_L \sum_{\hat{P} \Lambda n} dE_{cm}(L, \hat{P} \Lambda n; \{a\}) C^{-1}(L, \hat{P} \Lambda n; \hat{P} \Lambda n') dE_{cm}(L, \hat{P} \Lambda n'; \{a\}).
\]

Here

\[
dE_{cm}(L, \hat{P} \Lambda n; \{a\}) = E^\text{obs}_{cm}(L, \hat{P} \Lambda n) - E^\text{calc}_{cm}(L, \hat{P} \Lambda n; \{a\})
\]

is the difference between an observed lattice energy level \( E^\text{obs}_{cm}(L, \hat{P} \Lambda n) \) and the analytically calculated energy level.

\( \hat{P} \Lambda n \) and the analytically calculated energy level.
$E^{cm}_{n} (L, \vec{P}h; \{a\})$ that satisfies the generalized L"uscher's equation \cite{1,2}

$$\text{det}([\tilde{K}_{1sJl^2}^{(J)}(E_{cm}, \{a\})]^{-1} \delta_{JJ'} - \delta_{ss'} B^{(J)}_{JlJ'l} (E_{cm})] = 0 \quad (2)$$

for a given set of parameter values $\{a\}$. The $B$ is a known kinematical matrix, computed using the TwoHadronsInBox package \cite{3,4} and $K^{-1}(E_{cm}, \{a\})$ is related to $t$ as

$$(t^{(J)}_{1sJl^2})^{-1} = \frac{2(\tilde{K}_{1sJl^2}^{(J)}(E_{cm}, \{a\})^{-1} - 2p\dot{\delta}_{ss'} E_{cm} p'p''}.$$  \quad (3)

Here ($l$, $s$, $J$) refer to the partial-wave, the total spin and the total angular momentum of the incoming particles involved in the scattering, whereas the primed variables refer to that of the outgoing particles. The data covariance $C(L; \vec{P}h; P'L'n')$ is determined using the procedure outlined in Appendix A of Ref. \cite{5}. The solutions of the L"uscher's equation (2) are extracted by performing an eigenvalue decomposition of the matrix

$$\tilde{A}(E_{cm}) = \frac{A}{\text{det}( (\mu^2 + AA^t)^{1/2})}, \quad (4)$$

along the lines as discussed in Ref. \cite{6}. Here $A$ is the argument of determinant in Eqn. 2 and $\mu = 2.0$ is chosen throughout the calculation. We find our results are independent of the value of $\mu$ across a wide interval [0.1, 100].

Under the assumption that any contribution from $l \geq 2$ partial waves are negligible\footnote{All the energy levels with dominant overlap to operators with $l = 2$ partial waves are consistent with the respective non-interacting energies. Any contribution of $l \geq 2$ partial waves on the finite volume levels close to the $DD^*$ threshold, which is the energy region of interest, are suppressed by the phase space factor $p^3$. The extraction of any other effects from $l \geq 2$ partial waves need the utilization of larger volume ensembles, which is beyond the scope of this work.}, $K^{-1}(E_{cm}, \{a\})$ for elastic $DD^*$ scattering reduces to a $3 \times 3$ diagonal matrix, where elements are related to $t$ and $\delta$ as follows

$$(t^{(J)}_{1})^{-1} = \frac{2(\tilde{K}_{1sJl^2}^{(J)}(E_{cm}, \{a\})^{-1} - 2p\dot{\delta}_{ss'} E_{cm} p'p''}.$$  \quad (5)

We parametrize it with the effective range expansion

$$\tilde{K}^{-1} = \begin{bmatrix} \frac{1}{a_0} + \frac{x^{(1)} p^2}{2} & 0 & 0 \\ 0 & \frac{1}{a_1} + \frac{x^{(0)} p^2}{2} & 0 \\ 0 & 0 & \frac{1}{a_2} \end{bmatrix}.$$  \quad (6)

We perform separate and combined fits to the $JF(l) = 1^+(0), 0^-(1)$ channels (first two rows in the above $K^{-1}$ matrix) using $T_{11}$ and $A_{1}$ irrep s in the rest frame and $A_{2}$ irrep s in the moving frame with $\vec{P} = (0, 0, 1)\hat{z}$. Possible effects from the left-hand cuts are omitted. The fitting details, quality, results, and the parameter covariance for all fits in the two $m_c$ we studied are listed in Table 4. It is evident that the best fit parameters for $l = 0 \ DD^*$ scattering amplitude is stable with respect to separate and combined fits in the low energy region. $p\cot(\delta_0)$ as a function of $p^2$ is presented in Fig. 2 of the main text and Fig. 1 below for the $m_c^{(b)}$ and $m_c^{(l)}$, respectively.

![FIG. 1. $p\cot(\delta_{i=0})$ versus $p^2$ in units of $E_{DD^*} = m_D + m_{D^*}$ for $DD^*$ scattering at the light charm quark mass. The (cyan) orange dashed curve refers to the (virtual) bound state constraint. Green and blue circles indicate the simulated data, whereas the solid red curve along with the gray band are the fit results. The virtual bound state occurs at the momenta indicated by the magenta octagon, where red and cyan curves intersect.](image)

In order to affirm our findings, we analytically predict the finite-volume energies in all five irreps. For this, we assume the full form of the $\tilde{K}^{-1}$ matrix in Eq. (6) taking fit results with ID (2) and (4) in Table 4 and a small constant value for $a_{1}^{(2)}$ to imitate a non-interacting scenario in this channel. This is then compared with the simulated finite volume energies to assess the quality of prediction. The $\chi^2/dof$ evaluated using the predicted energies and the simulated results are 23/14 and 30/14 for the $m_c^{(b)}$ and $m_c^{(l)}$, and are presented in Fig. 1 of the main text and Fig. 1 below, respectively. We find that the pattern of predicted and simulated finite volume energies are consistent, as shown by the smaller and larger symbols in these figures. We also observe that expanding the $\tilde{K}^{-1}$ matrix to include nearly non-interacting $JF(l) = 1^+(2), 2^+(2)$ channels, also involving a possible mild partial wave mixing between $JF(l) = 1^+(0)$ and $JF(l) = 1^+(2)$ does not alter the finite-volume energies up to $E_{cm}/E_{DD^*} = 1.025$ and also leads to the same $\chi^2/dof$ value. In short, we find that our estimate for $DD^*$ scattering amplitude with $l = 0$ is robust to contaminations from other possible nearby channels.
TABLE I. Details and results of the scattering analysis: the partial waves considered, the finite-volume energies included, the quality, the best fit values and the covariances for the resulting parameters of various fits. In the last two columns, we also present the binding energy and a compositeness measure, as defined in Ref. [40], of the $l = 0$ virtual bound state.

| $m_c$ | ID | $\Lambda((P^2)^2)$ | $E^\text{lat}$ info | $\chi^2$/dof | a | a Covariance | $\delta m_{R_c}$ [MeV] | $\bar{X}_A$ |
|-------|----|-------------------|----------------------|-------------|---|--------------|---------------------|---------|
| 1.05Ecm/EDD * | 1 | $T_1^+(0)$ | (1000, 1100) | 1.3 | $a_0^{(1)} = 1.13(0.37, 0.22)$ fm $r_0^{(1)} = 0.94(0.20, 0.20)$ fm | 1.00 | 0.06 | -8.9(0.7) | 0.61(7) |
| 1.05Ecm/EDD * | 2 | $T_1^+(0)$ | (1000, 1100) | 3.7 | $a_0^{(1)} = 1.04(0.29)$ fm $r_0^{(1)} = 0.96(0.18, 0.20)$ fm $a_1^{(0)} = 0.076(0.009)$ fm$^3$ $r_1^{(0)} = 6.9(2.1)$ fm$^{-1}$ | 1.00 | 0.13 | -0.28 | -0.18 | -9.9(0.7) | 0.59(6) |
| 1.05Ecm/EDD * | 3 | $T_1^+(0)$ | (1000, 1100) | 1.4 | $a_0^{(1)} = 0.94(0.25)$ fm $r_0^{(1)} = 0.96(0.18, 0.20)$ fm | 1.00 | 0.06 | -0.02 | 0.02 | -12.9(0.8) | 0.57(6) |
| 1.05Ecm/EDD * | 4 | $T_1^+(0)$ | (1000, 1100) | 3.6 | $a_0^{(1)} = 0.86(0.22)$ fm $r_0^{(1)} = 0.92(0.17, 0.19)$ fm $a_1^{(0)} = 0.117(0.0013)$ fm$^3$ $r_1^{(0)} = 8.6(1.5)$ fm$^{-1}$ | 1.00 | 0.12 | -0.09 | -0.11 | -15.0(0.9) | 0.56(5) |

FIG. 2. Finite-volume energy levels ($E_{cm}$) in the center-of-momentum frame in units of $E_{DD^*} \equiv m_D + m_{D^*}$ for the lighter charm quark mass. The results from lattice simulation are shown by empty circles and squares: blue and green circles are employed in the extraction of $DD^*$ scattering amplitude with $l = 0, 1$. The non-interacting $DD^*$ energies (Eq. (1) in the main text) are shown by lines: the operators related to black lines are considered, while the those related to the gray lines are omitted from the calculation. [2] in $T_1^+(0)$ and $A_2(2)$ refers to the multiplicity of non-interacting level $D(1)D^*(1)$, in these irrep. The orange stars represent the analytically predicted energies based on the fitted scattering amplitudes and are slightly horizontally shifted for clarity.

III. DEPENDENCE OF BINDING ENERGY ON $m_{u/d}$ AND $m_c$

In this section we provide some simple quantum mechanic arguments that the pole position of $DD^*$ scattering in partial wave $l = 0$ roughly varies with changing $m_{u/d}$ or $m_c$ as sketched in Fig. 4 of the main article. We consider a pole related to the state dominated by a molecular Fock component. The pole positions found
by LHCb and by our lattice study at two charm quark masses are in line with these arguments. However, further lattice studies at various quark masses are needed to establish these arguments empirically.

We investigate position of the pole for purely attractive potential \( V(r) = -V_0 f(r) \) between \( D \) and \( D^* \) with \( V_0 > 0 \). We explored various shapes, for example the Yukawa \( f(r) = e^{-r/R}/r \), exponential \( f(r) = e^{-r/R} \), square-well \( f(r) = \theta(r_0 - R) \). For a given potential, we numerically determined the phase-shift \( \delta_0 \), the scattering amplitude and the energy, where scattering amplitude has a pole.

We focused on the potentials where the pole is close to the threshold. Fig. 3 shows a typical dependence of the pole position on varying one of the parameters in potential \( V_0, R \) or the reduced mass \( m_r \). The bound state is present for large attraction \( V_0 \). As \( V_0 \) is decreased, the binding energy of the bound state decreases, at critical \( V_0 \) it turns to a virtual bound state and then the pole moves further below threshold. Analogous behavior is observed when the reduced mass \( m_r \) is decreased or when the range of the potential \( R \) is increased. Note that the bound state does not turn to a resonance for a purely attractive potential since there is no repulsive centrifugal barrier for \( l = 0 \) to keep the resonance metastable. All shapes of the potentials we explored show these robust features.

Let us now consider how the quark masses affect the values of \( V_0, R, m_r \) and thereby the pole positions. As \( m_{u/d} \) increases, the mass of the exchanged light mesons \( M \) also increases and the range of the potential \( R \simeq 1/M \) decreases, which renders the dependence on \( m_{u/d} \) sketched in Fig. 4 of the main article. Here we assumed that the dependence of the reduced mass on \( m_{u/d} \) is negligible.

The decrease of \( m_c \) will decrease the reduced mass \( m_r \) of the \( DD^* \) system, while the potential will not change drastically due to the heavy quark flavor symmetry. The bound state becomes less and less bound with decreasing \( m_c \) and eventually turns to a virtual bound state.

Now let us turn to quark mass dependence of the bound state dominated by the diquark antidiquark Fock component \([QQ][\bar{u}\bar{d}]\). The attractive colour Coulomb potential between two heavy quarks in diquark \([QQ]\) is flavor blind, while the kinetic energy increases with decreasing \( m_Q \). This implies that the binding energy decreases with decreasing \( m_Q \). The attraction within the good light diquark \([ud]\) becomes less significant as \( m_{u/d} \) increases \cite{23}, which implies that the binding energy will decrease. This is in line with the sketch for the bound state behavior in Fig. 4 of the main article, which is supported by the phenomenological studies \cite{8, 10} and lattice studies of \( bb\bar{u}\bar{d} \) \cite{15, 20, 22}. However, it is not known from lattice simulations yet what is the fate of a pole when a diquark antidiquark state is on the verge of binding and whether it would turn to a resonance or virtual state. The analytical considerations of compositeness in Ref. \cite{40} suggest that compact states exist as bound states or resonances.