Evidence for $X(3872)$ from DD^* Scattering on the Lattice

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A candidate for the charmonium(like) state $X(3872)$ is found 11 ± 7 MeV below the $D\bar{D}^*$ threshold using dynamical $N_f = 2$ lattice simulation with $J^{PC} = 1^{++}$ and $I = 0$. This is the first lattice simulation that establishes a candidate for $X(3872)$ in addition to the nearby scattering states $D\bar{D}^*$ and $J/\psi\omega$, which inevitably have to be present in dynamical QCD. We extract large and negative $D\bar{D}^*$ scattering length $a_0^{DD^*} = -1.7 \pm 0.4$ fm and the effective range $r_0^{DD^*} = 0.5 \pm 0.1$ fm, but their reliable determination will have to wait for a simulation on a larger volume. In $I = 1$ channel, only the $D\bar{D}^*$ and $J/\psi\rho$ scattering states are found and no candidate for $X(3872)$. This is in agreement with the interpretation that $X(3872)$ is dominantly $I = 0$, while its small $I = 1$ component arises solely from the isospin breaking and is therefore absent in our simulation with $m_u = m_d$.

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The narrow charmonium(like) state $X(3872)$ with $m_X^{\rm exp} = 3871.68 \pm 0.17$ MeV [1] has been confirmed by many experiments since its discovery [2], but its quantum numbers have been unambiguously determined to be $J^{PC} = 1^{++}$ only very recently [3]. Experimentally, it is found within 1 MeV of the $D^0\bar{D}^{0*}$ threshold and has an interesting feature that it decays to isospin zero $J/\psi\omega$ as well as isospin one $J/\psi\rho$ states.

Theoretically, it has been addressed within a great number of phenomenological models (for review, see Refs. [4,5]). The $J^{PC} = 1^{++}$ charmonium channel with $I = 0$ has been simulated recently also in lattice QCD using only $\bar{c}c$ interpolating fields, where impressive J^{PC} identification was made in Ref. [6], the continuum and chiral extrapolations were considered in Refs. [7–9], while a recent review on charmonium results from lattice is given in Ref. [10]. However, $X(3872)$ has never been unambiguously identified from a lattice simulation yet. Several simulations [6,8,9,11] in fact found one state near $E \simeq m_X^{\rm exp}$, but it was impossible to unambiguously determine whether this state is $X(3872)$ or the scattering state $D\bar{D}^*$, which should in principle also appear as an energy level at very similar energy in a dynamical lattice QCD.

There was one simulation that employed $\bar{c}c$ as well as $D\bar{D}^*$ interpolating fields, but the results could not support or disfavor the existence of $X(3872)$, since only the lowest two energy levels in 1^{++} channel were extracted [12]. The same holds for Ref. [13], where only one level near the $D\bar{D}^*$ threshold was extracted using various four-quark interpolators. Examples of results for near-threshold bound states in other channels are presented in Refs. [14–20].

The purpose of our present simulation is to identify the low-lying $\chi_{c1}(1P)$ and $X(3872)$ as well as all the nearby discrete scattering levels $D\bar{D}^*$ and $J/\psi\omega$ for $I = 0$. The number of energy levels near $D\bar{D}^*$ threshold will indicate whether we observe a candidate for $X(3872)$ or not. We search for $X(3872)$ also in the $I = 1$ channel.

In lattice QCD simulations, the states are identified from discrete energy levels E_n and in principle, all physical eigenstates with the given quantum number appear. We employ $J^{PC} = 1^{++}$, $I = 0$ or $I = 1$ and total momentum zero. So the eigenstates are also the s-wave scattering states $D(\mathbf{p})\bar{D}^*(-\mathbf{p})$ and $J/\psi(\mathbf{p})V(-\mathbf{p})$ with discrete momenta $\mathbf{p}$ due to periodic boundary conditions in space, where $V = \omega$ for $I = 0$ and $V = \rho$ for $I = 1$. If the two mesons do not interact then $p = p^{\rm n.i.} = (2\pi/L)|\mathbf{n}|$ and the noninteracting (n.i.) scattering levels appear at $E^{\rm n.i.} = E_1(p^{\rm n.i.}) + E_2(p^{\rm n.i.})$. In the presence of interaction, the scattering levels $E = E_1(p) + E_2(p)$ are shifted with respect to $E^{\rm n.i.}$ since momentum p outside the interaction region is different from $p^{\rm n.i.} = (2\pi/L)|\mathbf{n}|$. This energy shift provides rigorous information on the $D\bar{D}^*$ interaction. Bound states and resonances lead to levels in addition to the scattering levels and our major task is to look for these additional levels.

Our simulation is based on one ensemble of Clover-Wilson dynamical and valence u, d quarks with $m_u = m_d$ and $m^{\rm val} = m^{\rm dyn}$, corresponding to $m_\pi = 266(4)$ MeV. The lattice spacing is $a = 0.1239(13)$ fm, the volume is $V = 16^3 \times 32$ and the small spatial size $L \simeq 2$ fm is the main drawback of our simulation considering that $X(3872)$ is probably large in size. Our exploratory results might therefore have sizable finite-volume corrections. The main purpose of this Letter is, however, counting the number of lattice states near $D\bar{D}^*$ threshold in order to establish the existence of $X(3872)$.

The charm quarks are treated using the Fermilab method [21], according to which $E - \frac{1}{4}(m_{0^-} + 3m_{1^-})$ are compared between lattice and experiment. The m_c is fixed by tuning the spin-averaged kinetic mass $\frac{1}{4}(m_{\eta_c} + 3m_{J/\psi})$ to its physical value [11]. We employed the same method on this ensemble and found good agreement with experiment for conventional charmonium spectrum as well as masses and widths of charmed mesons in Ref. [11]. The present study also needs the following masses for our ensemble: $am_D = 0.9801(10)$, $am_{D^*} = 1.0629(13)$, $am_{\eta_c} = 1.473\,92(31)$, $am_{J/\psi} = 1.541\,71(43)$ [11], $am_\rho = 0.5107(40)$, and $m_\omega \simeq m_\rho$ within errors.

The energy levels E_n and overlaps $Z_i^n \equiv \langle \mathcal{O}_i | n \rangle$ of eigenstates n are extracted from the correlation matrix

$$C_{ij}(t) = \langle \mathcal{O}_i^\dagger(t + t_{\rm src}) | \mathcal{O}_j(t_{\rm src}) \rangle = \sum_n Z_i^n Z_j^{n*} e^{-E_n t}, \quad (1)$$

which are averaged over every second $t_{\rm src}$. We choose interpolating fields $\mathcal{O}_i$ that couple well to $\bar{c}c$ as well as the scattering states to study the system with total momentum zero, $I = 0$ or $I = 1$, and $J^{PC} = 1^{++}$ (we employ irreducible representation T_1^{++} of the lattice symmetry group O_h, which contains $J^{PC} = 1^{++}$ and in general also $J^{PC} \geq 3^{++}$ states, but those are at least 200 MeV above the region of interest [11])

$$\begin{aligned}
O_{1-8}^{\bar{c}c} &= \bar{c}\hat{M}_i c(0), \quad (\text{only } I = 0) \\
O_1^{DD^*} &= [\bar{c}\gamma_5 u(0)\bar{u}\gamma_i c(0) - \bar{c}\gamma_i u(0)\bar{u}\gamma_5 c(0)] + f_I\{u \to d\}, \\
O_2^{DD^*} &= [\bar{c}\gamma_5\gamma_t u(0)\bar{u}\gamma_i\gamma_t c(0) - \bar{c}\gamma_i\gamma_t u(0)\bar{u}\gamma_5\gamma_t c(0)] \\
&\quad + f_I\{u \to d\}, \\
O_3^{DD^*} &= \sum_{e_k = \pm e_{x,y,z}} [\bar{c}\gamma_5 u(e_k)\bar{u}\gamma_i c(-e_k) \\
&\quad - \bar{c}\gamma_i u(e_k)\bar{u}\gamma_5 c(-e_k)] + f_I\{u \to d\}, \\
O_1^{J/\psi V} &= \epsilon_{ijk}\bar{c}\gamma_j c(0)[\bar{u}\gamma_k u(0) + f_I \bar{d}\gamma_k d(0)], \\
O_2^{J/\psi V} &= \epsilon_{ijk}\bar{c}\gamma_j\gamma_t c(0)[\bar{u}\gamma_k\gamma_t u(0) + f_I \bar{d}\gamma_k\gamma_t d(0)], \quad (2)
\end{aligned}$$

where $f_I = 1$ and $V = \omega$ for $I = 0$, while $f_I = -1$ and $V = \rho$ for $I = 1$. Eight $\mathcal{O}^{\bar{c}c}$ are listed in Table X of Ref. [11] and polarization $i = x$ is used. Momenta are projected separately for each meson current: $\bar{q}_1 \Gamma q_2(n) \equiv \sum_x e^{i2\pi nx/L} q_1(x, t)\Gamma q_2(x, t)$ All quark fields are smeared $q \equiv \sum_{k=1}^{N_v} v^{(k)} v^{(k)\dagger} q_{\rm point}$ [11,22] with $N_v = 96$ Laplacian eigenvectors for $O^{\bar{c}c}$, $\mathcal{O}_1^{DD^*}$, $\mathcal{O}_1^{J/\psi V}$, and $N_v = 64$ for the remaining three. The energy of $J/\psi(1)V(-1)$ is expected

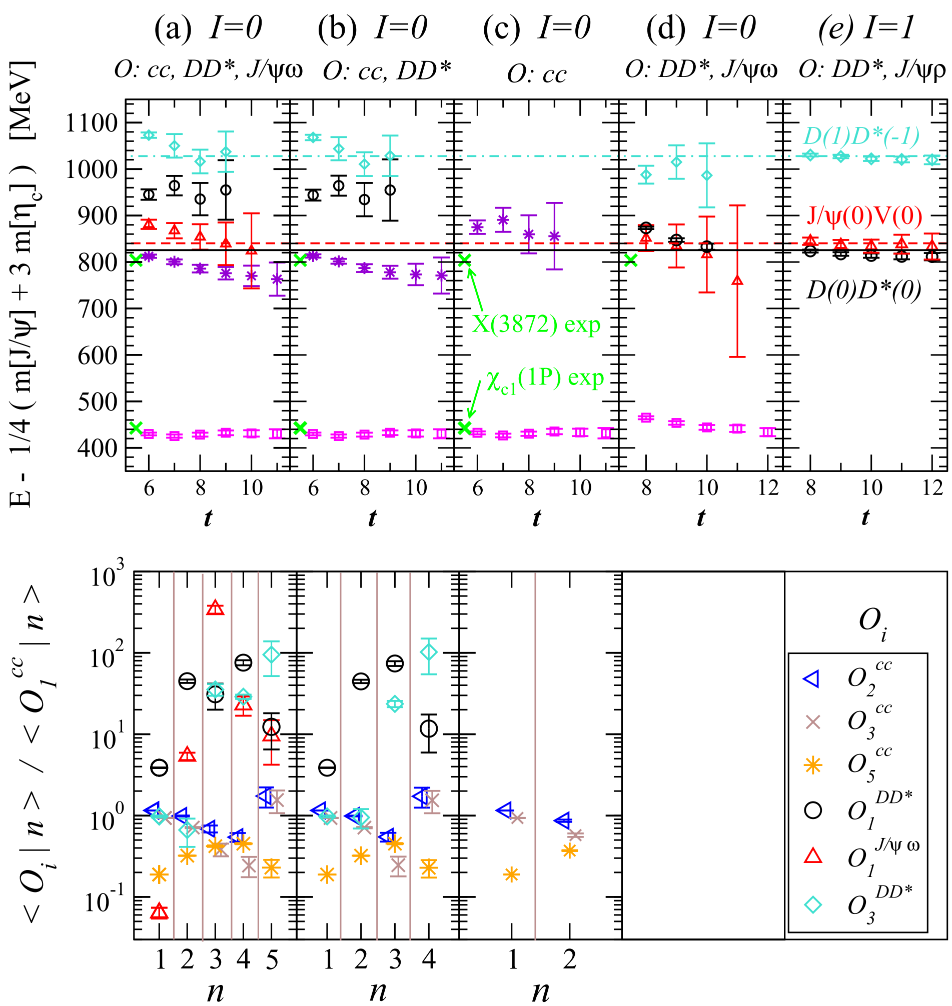

FIG. 1 (color online). Upper figure: symbols represent $E_n - \frac{1}{4}(m_{\eta_c} + 3m_{J/\psi})$ in the plateau region, where E_n are energies of the eigenstates n in the $J^{PC} = 1^{++}$ channel ($n = 1, 2, \ldots$ starting from the lowest state). The choice of the interpolator basis [Eq. (2)] is indicated above each plot. Dashed lines represent energies $E^{\rm n.i.}$ of the noninteracting scattering states. Lower figure: overlaps $\langle \mathcal{O}_i | n \rangle$ of eigenstates n (from the upper figure) with interpolators $\mathcal{O}_i$, all normalized to $\langle \mathcal{O}_1^{\bar{c}c} | n \rangle$. Note that all $\langle \mathcal{O}_i^{DD*,J/\psi\omega} | n \rangle / \langle \mathcal{O}_1^{\bar{c}c} | n \rangle$ depend on one (arbitrary) choice for the normalization of the current $\bar{q}_1 \Gamma q_2(n)$ with a given quark smearing. The plotted ratios correspond to choice presented in the main text.

at least 200 MeV above the region of interest, so the corresponding interpolator is not implemented.

We calculate all Wick contractions [Figs. 1(a) and 1(b) of the Supplemental Material [23]] to the correlation matrix $C_{ij}(t)$ (13×13 for $I = 0$ and 5×5 for $I = 1$) using the distillation method [22]. Certain charm annihilation contractions are found to be very noisy like in previous simulations. Their effect on $I = 0$ charmonium states is suppressed due to the Okubo-Zweig-Iizuka rule, it was explicitly verified to be very small in Ref. [24] and we postpone the study of their effects to a future publication. In the present Letter, we present results where $C_{ij}(t)$ contains all contractions, except for those where c quark does not propagate from source to sink [results are based on contractions in Fig. 1(a) of the Supplemental Material [23]].

The energies E_n and overlaps $\langle O_i|n\rangle$ are extracted from the time dependence of the correlation matrix $C_{ij}(t)$ using the generalized eigenvalue method $C(t)u_n(t) = \lambda_n(t)C(t_0)u_n(t)$ [25,26]. Results are consistent for range $2 \leq t_0 \leq 6$ and we present them for $t_0 = 2$, when the highest level is least noisy. The eigenvalues $\lambda_n(t) \to e^{-E_n(t-t_0)}$ give the effective energies $E_n^{\rm eff}(t) \equiv \log[\lambda_n(t)/\lambda_n(t+1)] \to E_n$ plotted in Fig. 1, which equal the energies E_n in the plateau region. Ratios of overlaps for state n to two different interpolators [26],

$$\frac{\langle \mathcal{O}_i|n\rangle}{\langle \mathcal{O}_j|n\rangle} = \frac{\sum_k C_{ik}(t)u_k^n(t)}{\sum_{k'} C_{jk'}(t)u_{k'}^n(t)}, \tag{3}$$

evaluated at $t = 8$ are also shown (they are obtained from the full interpolator basis but only few representative $\mathcal{O}_i$ are shown). We verify that ratios are almost independent of time for $6 \leq t \leq 10$, indicating that our eigenstates n in Fig. 1 do not change composition in time.

The main result of our simulation is the discrete spectrum for $J^{PC} = 1^{++}$ and $I = 0, 1$ in Fig. 1. According to the Fermilab method for treating charm quark, we are presenting the difference of E and the spin average $\frac{1}{4}(m_{\eta_c} + 3m_{J/\psi})$ [11], both evaluated from simulation. The horizontal lines represent energies of the noninteracting scattering states $E^{n.i.}$ on our lattice.

Results for $I = 1$.—This channel cannot contain pure $\bar{c}c$. The lowest three levels are $D(0)\bar{D}^*(0)$, $J/\psi(0)\rho(0)$, and $D(1)\bar{D}^*(-1)$, and we verify that their overlaps are indeed largest with $\mathcal{O}_{1,2}^{DD^*}$, $\mathcal{O}_{1,2}^{J/\psi\rho}$, and $\mathcal{O}_3^{DD^*}$, respectively. Their energies are almost equal to noninteracting energies $E^{\rm n.i.}$ represented by the horizontal lines, which indicates that the interaction in $I = 1$ channel is small. We find no extra state in addition to the scattering states in the $I = 1$ channel, thus, no candidate state for $X(3872)$.

The sizable decay $X(3872) \to J/\psi\rho$ in experiment makes this state particularly interesting and gives rise to two popular interpretations. Both are based on the isospin breaking with the dominant effect coming from the 8 MeV isospin splitting of the $D^0\bar{D}^{0*}$ and $D^+\bar{D}^{-*}$ [27,28]. The first interpretation is based on $X(3872)$ with $I = 0$ and the isospin is broken in the decay. The second possibility is that $X(3872)$ is a linear combination $|X(3872)\rangle = a_{I=0}|DD^*\rangle_{I=0} + a_{I=1}|DD^*\rangle_{I=1}$ with $a_{I=1} \ll a_{I=0}$ and $a_{I=1}(m_u = m_d) = 0$ [27,28]. Our nonobservation of $X(3872)$ with $I = 1$ is in agreement with both interpretations due to exact isospin with $m_u = m_d$ in our simulation. Another possibility is that five $I = 1$ scattering interpolators [Eq. (2)] are not diverse enough to render $X(3872)$, which calls for simulations including also other types of $I = 1$ interpolators in the future.

Results for $I = 0$.—The lowest energy state in Fig. 1 is the conventional $\chi_{c1}(1P)$. The energy state represented by the triangles is $J/\psi(0)\omega(0)$; it disappears if $\mathcal{O}_{1,2}^{J/\psi\omega}$ is not used in the basis of $C_{ij}(t)$, leaving the remaining energies and overlaps almost unmodified [Fig. 1(b)], which indicates that $J/\psi\omega$ is not significantly coupled to the rest of the system. The diamonds correspond to $D(1)D^*(-1)$ and have largest overlap to $\mathcal{O}_3^{DD^*}$.

There are two remaining levels (circles and stars) in Figs. 1(a) and 1(b) and one of them has to be $D(0)\bar{D}^*(0)$. The other level is an evidence for the presence of a physical state in the energy region near $D\bar{D}^*$ threshold and we believe it is related to experimental $X(3872)$. We emphasize again that no lattice simulation has found evidence for $X(3872)$ in addition to the scattering states yet.

One expects two possible interpretations of the energy levels with circles and stars in Figs. 1(a) and 1(b), but the quantitative analysis rules out the second option.

1. Stars correspond to a weakly bound state $X(3872)$ slightly below $D\bar{D}^*$ threshold and circles correspond to the scattering state $D(0)\bar{D}^*(0)$, which is significantly shifted up due to a large negative $D\bar{D}^*$ scattering length $a_0^{DD^*} \equiv \lim_{p\to 0}\tan(p)/p$.

This is exactly a scenario envisaged for one shallow bound state on the lattice [15] and confirmed for deuteron in Refs. [19,20]. Levinson's theorem requires the $D\bar{D}^*$ phase shift to start at $\delta(p = 0) = \pi$ and fall down to $\delta(p \to \infty) = 0$ for one near-threshold bound state. This implies negative $a_0^{DD^*}$ and positive energy shift of $D(0)\bar{D}^*(0)$ [29].

2. The other possibility would be to identify the circles with a resonance above $D\bar{D}^*$ threshold and stars with the down-shifted $D(0)\bar{D}^*(0)$ scattering level arising from the attractive interaction with positive $a_0^{D\bar{D}^*}$. This interpretation is however ruled out for our data which leads to $a_0^{DD*} < 0$ in Eq. (6) below.

We conclude that $X(3872)$ is related to the energy level indicated by stars in Figs. 1(a) and 1(b).

An interesting question is whether $X(3872)$ is accompanied by slightly heavier state, sometimes called $\chi_{c1}(2P)$, with the same quantum numbers. Figure 1(a) shows that we do not find a candidate for such a state for $E < 4100$ MeV, in agreement with experiment which also fails to

TABLE I. The energies extracted from the one-exponential correlated fit of the $6 \times 6\, C_{ij}(t)$ based on $O^{\bar{c}c}_{1,3,5}$, $\mathcal{O}^{DD^*}_{1,2,3}$, and $t_0 = 2$. The p denotes D and D^* momentum and $\delta(p)$ denotes their scattering phase shift.

Level n	Fit t	$E_n - \frac{1}{4}(m_{\eta_c} + 3m_{J/\psi})$ [MeV]	p^2 [GeV^2]	$p \cdot \cot\delta(p)$ [GeV]
1	6–11	429(3)		
2	8–11	785(8)	−0.075(15)	−0.21(5)
3	6–9	946(11)	0.231(22)	0.17(9)
4	7–10	1028(18)		

find another 1^{++} state nearby. Our results therefore allow the possibility for interpreting $X(3872)$ as $\chi_{c1}(2P) = \bar{c}c$ accidentally aligned with $D\bar{D}^*$ threshold.

We find $\chi_{c1}(1P)$ but no candidate for $X(3872)$ in $I = 0$ channel if the interpolator basis consists only of five scattering interpolators [Fig. 1(d)]. Perhaps this can be understood if $X(3872)$ is a consequence of accidental alignment of the $c\bar{c}$ state with $D\bar{D}^*$ threshold, which may be absent in practice if $\mathcal{O}^{\bar{c}c}$ are not explicitly incorporated.

The phase shifts $\delta(p)$ for the s-wave $D\bar{D}^*$ scattering are extracted using the well-established and rigorous Lüscher's relation [29],

$$p \cdot \cot\delta(p) = \frac{2Z_{00}(1; q^2)}{\sqrt{\pi}L}, \qquad q^2 \equiv \left(\frac{L}{2\pi}\right)^2 p^2, \tag{4}$$

which applies for elastic scattering below and above threshold. The D and $\bar{D}^*$ momentum p is extracted from $E_n = E_D(p) + E_{D^*}(p)$ using dispersion relations $E_{D,D^*}(p)$ [11] and $E_{n=2,3}$ from Fig. 1(b) and Table I. These energies result from correlation matrix with $\mathcal{O}^{\bar{c}c}$, $\mathcal{O}^{DD^*}$ but without $\mathcal{O}^{J/\psi\omega}$, so we expect that the effect of the $J/\psi\omega$ is negligible. This is confirmed by comparing Figs. 1(a) and 1(b).

The resulting $p\cot\delta$ in Table I for p^2 slightly below and above threshold can be described by the effective range approximation for $D\bar{D}^*$ scattering in s wave,

$$p\cot\delta(p) = \frac{1}{a_0^{DD*}} + \frac{1}{2} r_0^{DD*} p^2. \tag{5}$$

Inserting $p\cot\delta(p)$ and p^2 for levels $n = 2, 3$ to Eq. (5), we get two relations which render the $(D\bar{D}^*)_{I=0}$ scattering length and the effective range at our $m_\pi \simeq 266$ MeV,

$$a_0^{DD^*} = -1.7 \pm 0.4 \text{ fm}, \qquad r_0^{DD^*} = 0.5 \pm 0.1 \text{ fm}. \tag{6}$$

The infinite volume $D\bar{D}^*$ bound state (BS) appears where S matrix, $S \propto (\cot\delta(p) - i)^{-1}$, has a pole, so for the value of $p^2_{\rm BS} < 0$ where $\cot\delta(p_{\rm BS}) = i$. The $D\bar{D}^*$ bound state $X(3872)$ appears near threshold, so we determine the binding momentum $p^2_{\rm BS} = -0.020(13)$ GeV^2 which corresponds to $\cot\delta(p_{\rm BS}) = i$ from the effective range approximation [Eq. (5)] and the parameters [Eq. (6)]. This binding momentum then renders the position of the bound state $X(3872)$ in the infinite volume via $m_X^{\rm lat}(L \to \infty) = E_D(p_{\rm BS}) + E_{D^*}(p_{\rm BS})$ and the resulting mass in Table II is rather close to the experimental value. We used $D^{(*)}$ masses and dispersion relations $E_{D^{(*)}}(p)$ from Ref. [11], where they are extracted for employed configurations.

TABLE II. $m_{X(3872)}$ from lattice and experiment [1,30].

$X(3872)$	$m_X - \frac{1}{4}(m_{\eta_c} + 3m_{J/\psi})$	$m_X - (m_{D^0} + m_{D^{0*}})$
Lattice$^{L\to\infty}$	815 ± 7 MeV	-11 ± 7 MeV
Experiment	804 ± 1 MeV	-0.14 ± 0.22 MeV

The errors correspond to statistical errors based on single-elimination jackknife. The largest systematic uncertainty is expected from the finite volume corrections and we estimate that m_X on the DD^* threshold is also allowed within our systematic errors, while m_X above threshold is not supported due to $a_0^{DD*} < 0$ [Eq. (6)]. Simulations on larger volumes will have to be performed to get more reliable result for $m_X - m_D - m_{D^*}$, and the prospects are discussed in the Supplemental Material [23]. The variation of m_X with $m_\pi = [140, 266]$ MeV is within this uncertainty according to the analytic study based on the molecular picture [31].

Concerning the composition of our candidate for $X(3872)$, Figure 1 shows its representative overlaps $\langle \mathcal{O}_i | n = 2\rangle$. It has particularly sizable overlaps with $\bar{c}c$ and $D(0)\bar{D}^*(0)$ interpolators, and has nonvanishing overlaps with the remaining ones. Note that the aim of the present Letter was not to choose between most popular interpretations ($\bar{c}c$ state accidentally aligned with DD^* threshold or $D\bar{D}^*$ molecule, etc.), but rather to find a candidate for $X(3872)$ on the lattice and determine its mass.

In conclusion, a candidate for $X(3872)$ is found 11 ± 7 MeV below the $D\bar{D}^*$ threshold using two-flavor dynamical lattice simulation with $J^{PC} = 1^{++}$ and $I = 0$. In the simulation, the $X(3872)$ appears in addition to the nearby $D\bar{D}^*$ and $J/\psi\omega$ discrete scattering states, and we extract large and negative $D\bar{D}^*$ scattering length. We do not find a candidate for $X(3872)$ in the $I = 1$ channel, which may be related to the exact isospin in our simulation.

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