Structure of the $X(3872)$ as explained by a diffusion Monte Carlo calculation

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Two decades after its unexpected discovery, the properties of the $X(3872)$ exotic resonance are still under intense scrutiny. In particular, there are doubts about its nature as an ensemble of mesons or having any other internal structure. We use a diffusion Monte Carlo method to solve the many-body Schrödinger equation that describes this state as a $c\bar{c}n\bar{n}$ ($n = u$ or d quark) system. This approach accounts for multiparticle correlations in physical observables avoiding the usual quark-clustering assumed in other theoretical techniques. The most general and accepted pairwise Coulomb + linear-confining + hyperfine spin-spin interaction, with parameters obtained by a simultaneous fit of around 100 masses of mesons and baryons, is used. The $X(3872)$ contains light quarks whose constituent masses are given by the dynamical breaking of chiral symmetry. The same mechanism gives rise to Goldstone-boson exchange interactions between light quarks whose contribution, derived from a well extended chiral quark model, has been included in this analysis but plays a marginal role. It appears that a meson-meson molecular configuration is preferred but, contrary to the usual assumption of $D^0\bar{D}^{*0}$ molecule for the $X(3872)$, our formalism produces $\omega J/\psi$ and $\rho J/\psi$ clusters as the most stable ones, which could explain in a natural way all the observed features of the $X(3872)$.

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I. INTRODUCTION

A very successful classification scheme for hadrons in terms of their valence quarks and antiquarks was independently proposed by Murray Gell-Mann [1] and George Zweig [2] in 1964. This classification was called the quark model, and it basically separates hadrons in two big families: mesons (quark-antiquark) and baryons (three-quark). The quark model received experimental verification beginning in the late 1960s and, despite extensive experimental searches, no unambiguous candidates for exotic configurations were identified until the turn of this century, with the discovery by the Belle Collaboration in 2003 [3] of the $X(3872)$ in the invariant mass spectrum of $\pi^+\pi^- J/\psi$ produced in $B^\pm \to K^\pm X(3872) \to K^\pm(\pi^+\pi^- J/\psi)$ decays. Since then, more than two dozens of unconventional charmonium- and bottomoniumlike states, the so-called XYZ mesons, have been observed at B-factories (*BABAR*, Belle and CLEO), τ-charm facilities (CLEO-c and BESIII) and also proton-(anti)proton colliders (CDF, D0, LHCb, ATLAS, and CMS). For an extensive presentation of the status of heavy quarkonium physics, the reader is referred to several reviews [4–9].

Even today, the $X(3872)$ represents a puzzle with no consensus about its structure. Its current world average mass is (3871.69 ± 0.17) MeV [10], very similar to that of the charmed meson pair: $m(D^0\bar{D}^{*0}) = (3871.69 \pm 0.07)$ MeV. This state seems also extremely narrow with a width less than 1.2 MeV at 90% confidence level [10]. Experimental analysis from Belle and CDF collaborations, which combine angular information and kinematic properties of the $\pi^+\pi^-$ pair, strongly favor the quantum numbers $J^{PC} = 1^{++}$ [11–13]. The Review of Particle Physics (RPP) of the Particle Data Group (PDG) [10] has denoted this state as $\chi_{c1}(3872)$ with the following quantum numbers $I^G(J^{PC}) = 0^+(1^{++})$; however, experimental evidences in favor of the existence of $X(3872)$'s isovector partners have been pointed out very recently by the Belle Collaboration in Ref. [14], see also the contributions by Guskov on behalf of the COMPASS Collaboration [15,16].

From constituent quark models [17–19], the predicted masses of the $J^{PC} = 1^{++}$ $c\bar{c}$ low-lying states do not fit the one of the $X(3872)$. Nonetheless, the strongest evidence against a $c\bar{c}$ assignment for the $X(3872)$ is the fact that the dipion mass distribution in the $X(3872) \to \pi^+\pi^- J/\psi$ process proceeds through the $X(3872)$ decaying into a $\rho^0 J/\psi$ final state [3,12], which would violate isospin conservation if the $X(3872)$ were interpreted as a conventional charmonium state.

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The interpretation of $X(3872)$ as a molecular bound state with a very small binding energy [6,20–26] is favored by the closeness of the $X(3872)$'s mass and the $D^0\bar{D}^{*0}$ threshold. The ratio [10]

$$\mathcal{R}_{\omega-\rho} \equiv \frac{\mathcal{B}(X(3872) \to \pi^+\pi^-\pi^0 J/\psi)}{\mathcal{B}(X(3872) \to \pi^+\pi^- J/\psi)} = 1.1 \pm 0.4, \quad (1)$$

measured by Belle [11], *BABAR* [27] and BESIII [28], despite being well understood if the $X(3872)$ is interpreted as a DD^* molecular state, is not well reproduced in theoretical calculations, e.g., $\mathcal{R}_{\omega-\rho} \approx 0.15$ in Ref. [29]. This, together with the observation of $X(3872)$ decaying electromagnetically into $\gamma J/\psi$ and $\gamma\psi(2S)$ final states, could be interpreted as an indication that there is, at least, a significant mixing of the $c\bar{c}$ component with the $D^0\bar{D}^{*0}$ molecule; actually, there are theoretical works exploring such possibility in the market [30–33].

At this point, it seems clear that $X(3872)$ is not a charmonium state. Its minimal content must be then 4 quarks, i.e., a tetraquark system, an interpretation that was first proposed by Maiani *et al.* [34]. Under that prism, the $X(3872)$ could appear as a bound state of a diquark-antidiquark cluster. This was based on the idea that diquarks can be treated as a confined quasiparticles and used as degrees-of-freedom in parallel with quarks themselves [35–39]. However, the drawback of the tetraquark picture is the proliferation of the predicted states [34] and the lack of selection rules that may explain why many of these states are not seen [40,41].

In this manuscript we aim to elucidate the nature of the $X(3872)$ considering it as a tetraquark, specifically a $c\bar{c}n\bar{n}$ system, with n labeling either u- or d-quark. Unlike other former studies, we are not going to assume any particular clustering between the valence quarks (antiquarks). Moreover, the interaction between them is the most simple and accepted one: Coulomb+linear-confining+hyperfine spin-spin [42,43], supplemented by general expressions of pseudo-Goldstone exchange interactions between light quarks due to dynamical breaking of chiral symmetry [19,44–46].

It is worth highlighting that the set of model parameters were fitted in advance to reproduce a certain number of hadron observables within a given range of agreement with experiment. Therefore, it is difficult to assign an error to those parameters and, as a consequence, to the magnitudes calculated when using them. As the range of agreement between theory and experiment is around 10%–20%, this value can be taken as an estimation of the model uncertainty.

The many-body Schrödinger equation including all the 2-body potential terms mentioned above is solved by a diffusion Monte Carlo (DMC) technique which, in contrast with variational methods, considers in full the correlations between the particles of the system, and it is able to produce exactly the lowest eigenenergy of the system if a reasonable *ansatz* for its wave function is provided, instead of assuming any basis expansion of it.

II. THEORETICAL FORMALISM

Quantum Monte Carlo (QMC) methods have been successfully applied to many research areas such as quantum chemistry and material science [47–49]. However, the use of QMC techniques to hadron physics has been scarce, basically because these methods are ideally suited to answer questions related with many-body physics and most known hadrons consist on 2- and 3-body bound states. This paradigm is changing in the last twenty years with many experimental signals indicating the possibility of having a zoo of tetra-, penta- and even hexa-quark systems [10].

Carlson *et al.* [50,51] applied for the first time a variational quantum Monte Carlo (VQMC) algorithm, originally designed for nuclear physics problems, to the spectra of mesons and baryons. Their results compared reasonably well with those of the well-known Isgur-Karl's quark model [52–55]. Since that exploratory work, there was almost no related activity until 2020 when we used a DMC algorithm to calculate the full spectrum of fully-heavy tetraquark systems [56]. It is fair to notice that a DMC method was used to calculate the ground state energy of the $J^{PC} = 0^{++}$ $bb\bar{b}\bar{b}$ system by Bai *et al.* in 2019 [57]; however, important differences with respect our full analysis of all-heavy tetraquarks in Ref. [56] must be mentioned: (i) meson-meson and diquark-antidiquark clusters were assumed, (ii) the sextet-antisextet diquark-antidiquark configuration was fully neglected, and (iii) the hyperfine spin-spin interaction was computed perturbatively.

We follow the formalism of Ref. [56], and solve the 4-body Schrödinger equation that includes all the potential terms defined above for describing the $J^{PC} = 1^{++}$ $c\bar{c}n\bar{n}$ system, with n being either u- or d-quark, in both the isoscalar and isovector channels.

III. RESULTS

The binding energies for the $J^{PC} = 1^{++}$ $c\bar{c}n\bar{n}$ system in the isoscalar and isovector sectors are, respectively, −468 MeV and −460 MeV, which correspond to the absolute masses 3834 MeV and 3842 MeV. Note that these masses are below the DD^*, $\rho J/\psi$ and $\omega J/\psi$ theoretical thresholds, located at 3879 MeV, 3871 MeV and 3870 MeV, each in order. As in Ref. [43], the used quark masses are $m_u = 315$ MeV and $m_c = 1836$ MeV; they can be fine-tuned in order to get agreement with the experimental mass of the $X(3872)$. In any case, the model uncertainty allows well to assert that theoretical and experimental masses are in fair agreement.

In order to discern how sensible is our prediction with respect to different aspects of the phenomenological potential, the upper panel of Table I shows the predicted

TABLE I. Upper panel: masses, in MeV, of the mesons involved in this analysis and our tetraquark predictions considering two different situations: full calculation (M_f), and turning off the Goldstone-boson exchange potentials (M_χ). Experimental data are taken from Ref. [10]. Bottom panel: mass splitting, in MeV, between our tetraquark prediction and the relevant meson-meson thresholds in the original case (full) and when the color linear confining interaction is effectively screened ($\mu = 0.5, 1.0, 2.0\ \mathrm{fm}^{-1}$). See text for details.

	M_e [10]	M_f	M_χ
ρ	775	770	770
ω	783	769	770
D	1868	1863	1863
D^*	2009	2016	2016
J/ψ	3097	3101	3101
$c\bar{c}u\bar{u}$ $(I=0)$	⋯	3834	3874
$c\bar{c}u\bar{u}$ $(I=1)$	⋯	3842	3874

μ (fm^{-1})	Full	0.5	1.0	2.0
$M_{c\bar{c}u\bar{u}(I=0)} - M_{DD^*}$	−45	−65	−80	−96
$M_{c\bar{c}u\bar{u}(I=0)} - M_{\omega J/\psi}$	−36	−26	−15	−4
$M_{c\bar{c}u\bar{u}(I=1)} - M_{DD^*}$	−37	−54	−76	−94
$M_{c\bar{c}u\bar{u}(I=1)} - M_{\rho J/\psi}$	−29	−15	−11	−1

masses, in MeV, of the mesons involved in this analysis when considering the full potential (M_f) and turning off the Goldstone-boson exchange interactions (M_χ). One can see that our theoretical predictions are in fair agreement with experiment in all quark sectors: light-light, heavy-light, and heavy-heavy, indicating that one should expect a reasonable description of conventional hadrons when using our phenomenological potential.

Continuing with the upper panel of Table I, the same analysis has been performed for the tetraquark structures. One can see that the Goldstone-boson exchange interactions between light quarks play a marginal role. That is to say, when turning them off, the binding energy of the tetraquark system changes by less than 10%. This indicates that the most general and accepted quark-(anti)quark interaction, Coulomb + linear-confining + hyperfine spin-spin, is behind the dynamics of the tetraquark. It is also important to emphasize that the isoscalar and isovector $J^{PC} = 1^{++}$ $c\bar{c}n\bar{n}$ structures are clearly bounded even when the chiral contribution is disconnected; however, one can see in the upper panel of Table I that the tetraquark masses in such scheme are located below the DD^* threshold but slightly above the $\rho J/\psi$ and $\omega J/\psi$ ones.

The bottom panel of Table I explores how sensible are our results in terms of the large distance behavior of the confining interaction. Keeping all the remaining potentials in their original form, the confining term:

$$V^{(a)}_{\mathrm{CON}}(r,\lambda) = \lambda r, \tag{2}$$

has been replaced by

$$V^{(b)}_{\mathrm{CON}}(r;\lambda,\mu) = \frac{\lambda}{\mu}(1 - e^{-\mu r}), \tag{3}$$

where the parameter μ controls the transition regime between the linear behavior at short interquark distances and the regime in which the screening of the color confinement appears due to light quark-antiquark pair creation [58–60]. Moreover, this screening of the confinement potential allows us to bring artificially the mass of the tetraquark closer to the ones of the relevant meson-meson thresholds in order to discern whether it is a deeply bound, a loosely bound, or a scattering state.

The bottom panel of Table I shows the mass splitting, in MeV, between our tetraquark prediction and the relevant meson-meson thresholds in the original case (full, corresponding to $\mu \to 0$) and when the color linear confining interaction is effectively screened ($\mu = 0.5, 1.0, 2.0\ \mathrm{fm}^{-1}$). One can see that the tetraquark masses are in all cases located below the relevant meson-meson thresholds. However, it is fair to recognize that our tetraquark solutions, despite being deeply bound with respect to the DD^* threshold, gradually approach to the $\rho J/\psi$ and $\omega J/\psi$ ones.

We are now interested on elucidating the nature of the $J^{PC} = 1^{++}$ $c\bar{c}n\bar{n}$ structures obtained above and thus we exploit the concept of radial distribution function because it provides valuable information of the existence of interquark correlations; in particular, 2-body correlations. If the n-particle wave function is defined as $\psi(\vec{r}_1, \ldots, \vec{r}_n)$, where spin, flavor and color degrees of freedom have been ignored for simplicity without loss of generality, the probability of finding particle 1 in position $\vec{r}_1$, particle 2 in position $\vec{r}_2$,…, particle n in position $\vec{r}_n$ is:

$$P(\vec{r}_1, \ldots, \vec{r}_n) = \psi^*(\vec{r}_1, \ldots, \vec{r}_n)\psi(\vec{r}_1, \ldots, \vec{r}_n), \tag{4}$$

and it is normalized to one, i.e.,

$$1 = \int d\vec{r}_1 \cdots d\vec{r}_n P(\vec{r}_1, \ldots, \vec{r}_n). \tag{5}$$

Therefore, one can define

$$\rho^{(2)}(\vec{r}_1, \vec{r}_2) = \int d\vec{r}_3 \cdots d\vec{r}_n\, P(\vec{r}_1, \ldots, \vec{r}_n), \tag{6}$$

which expresses the probability of finding 2 particles in positions $\vec{r}_1$ and $\vec{r}_2$; and the radial distribution function as

$$\rho(r) = 4\pi r^2 \int d\vec{R}\rho^{(2)}(\vec{R} + \vec{r}, \vec{R}), \tag{7}$$

where r indicates now the distance between the two particles considered.

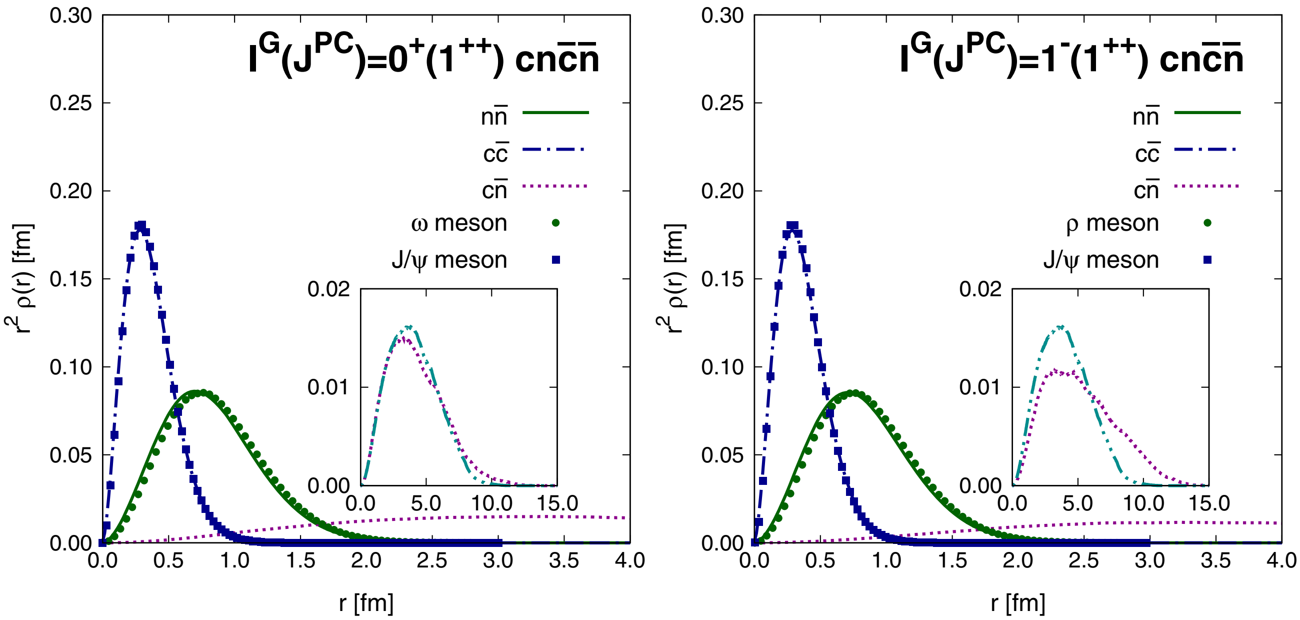

FIG. 1. Radial distribution functions (see text for details) for the studied $X(3872)$ candidate as either $I^G(J^{PC}) = 0^+(1^{++})$ (left panel) or $I^G(J^{PC}) = 1^-(1^{++})$ (right panel) $c\bar{c}n\bar{n}$ tetraquark bound-state. These functions represent the probability of finding the 2 quarks (antiquarks) at an interquark distance r. In both panels, solid (green), dot-dashed (blue) and dotted (purple) represent, respectively, $n\bar{n}$, $c\bar{c}$ and $c\bar{n}$ correlations inside the $c\bar{c}n\bar{n}$ tetraquark. The dot (green) and square (blue) points stand for the same object but calculated for the corresponding mesons, *i.e.,* $\omega - J/\psi$ for the left panel and $\rho - J/\psi$ for the right panel. The insets in each panel enlarge the range of the abscissa in order to appreciate that the $c\bar{n}$ correlation falls toward zero with respect to the interquark distance; moreover, an extra dot-dot-dashed (cyan) curve is added, indicating that the effect of decoupling the chiral potential does not change significantly the nature of the correlations observed in our tetraquark solutions. The other curves do not experience an appreciable modification if the Goldstone-boson exchange interaction is disconnected.

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Looking at the results shown in Fig. 1, one can conclude: (i) the $J^{PC} = 1^{++}$ $c\bar{c}n\bar{n}$ tetraquark tends to cluster in a meson-meson configuration and not in a diquark-antidiquark one; (ii) both quark-antiquark correlations have an extension $\lesssim$1 fm, separated by a distance of around 3 fm; (iii) the preferred arrangement is the one for which the quarks appear as a $(n\bar{n}) - (c\bar{c})$ pair of clusters, contrary to the general accepted $(n\bar{c}) - (c\bar{n})$ one due to the closeness of the $X(3872)$'s mass to the $D^0\bar{D}^{*0}$ threshold; (iv) the $n\bar{n}$ correlation resembles closely the omega (rho) meson in the isospin zero (one) sector, the $c\bar{c}$ correlation is clearly a J/ψ meson; and (v) $n\bar{n}$, $c\bar{c}$ and $c\bar{n}$ correlations fall off to zero with the interquark distance, indicating the fact of having finite size for the calculated tetraquark $c\bar{c}n\bar{n}$ structures. All of this may favor the light-meson–heavy-meson molecular bound-state picture for the $X(3872)$.[1]

It should be mentioned that our recent study on the lowest-lying states of all-heavy tetraquark systems [56] presents a similar feature in the quark-quark correlations of the $J^{PC} = 1^{++}$ $cb\bar{c}\bar{b}$ ground state (see left-bottom panel of Fig. 7 in Ref. [56]). The radial distribution

[1]It is worth mentioning that very extended molecular bound states with sizes larger than the typical interaction length between their constituents can be found in Nature; an example in QCD is the deuteron with a root mean square radius ≈2 fm, but a more striking one is the experimentally observed ^{4}He dimer whose radius is several tens of angstroms [61].

functions of the $J^{PC} = 1^{++}$ $cb\bar{c}\bar{b}$ ground state reveal that this state prefers to be organized in clusters of $c\bar{c}$ and $b\bar{b}$, whose extensions are less than 0.5 fm, separated by a distance of about 0.8–1.0 fm. However, the arrangement of quarks (antiquarks) in the $J^{PC} = 1^{++}$ $cb\bar{c}\bar{b}$ system is not repeated by its tetraquark partners with different quantum numbers $J^{PC} = 0^{++}$, 1^{+-}, and 2^{++}; neither seen in any other case of fully heavy tetraquarks explored in Ref. [56]: $cc\bar{c}\bar{c}$, $bb\bar{b}\bar{b}$, $cc\bar{b}\bar{b}$ ($bb\bar{c}\bar{c}$), $cc\bar{c}\bar{b}$, and $bb\bar{c}\bar{b}$.

The DMC formalism introduced in Ref. [56] allows us to compute not only the eigenenergy but also its associated wave function. In this case, we obtain[2]:

$$|X(3872)\rangle_{\mathrm{color}} = c_1|\bar{3}_{nc}3_{\bar{n}\bar{c}}\rangle_{\mathrm{color}} + c_2|6_{nc}\bar{6}_{\bar{n}\bar{c}}\rangle_{\mathrm{color}}, \quad (8)$$

with $c_1 \approx 0.57(1)$ and $c_2 \approx 0.82(1)$, in both isoscalar and isovector $J^{PC} = 1^{++}$ channels. Looking at Eqs. (56) and (57) of Ref. [56], our color wave function is essentially

$$|X(3872)\rangle_{\mathrm{color}} \approx |1_{c\bar{c}}\bar{1}_{n\bar{n}}\rangle_{\mathrm{color}}, \quad (9)$$

indicating that the computed tetraquark structures prefer to be in $(n\bar{n}) - (c\bar{c})$ configurations.[3] This supports the information related with the radial distribution functions shown in Fig. 1, therein we report an extra piece of information, i.e., such $n\bar{n}$ and $c\bar{c}$ correlations closely resemble either ω or ρ mesons, in the light sector, and J/ψ for the hidden-charm one.

Based on all the data above, our interpretation of the $X(3872)$ signal is that either two $c\bar{c}n\bar{n}$ loosely lying states with quantum numbers $I^G(J^{PC}) = 0^+(1^{++})$ and $1^-(1^{++})$, respectively, or just the same two but coupled together may explain all the observed features of the $X(3872)$. A meson-meson molecular configuration is preferred but, contrary to the usual assumption of having $D\bar{D}^*$ molecule, our formalism produces $\omega J/\psi$ and $\rho J/\psi$ clusters which could explain (i) the $X(3872)$'s discovery decay channel $\pi^+\pi^- J/\psi$, despite violating isospin conservation; (ii) the ratio $R_{\omega-\rho} \approx 1$ measured by different experimental collaborations worldwide; (iii) the observed radiative decay rates $\gamma J/\psi$ and $\gamma\psi(2S)$, incompatible with $D\bar{D}^*$-molecular interpretation, driven by the vector meson dominance mechanism, and (iv) production rates of the $X(3872)$ which are consistent with having a $c\bar{c}$ cluster.

IV. CONCLUSIONS

We use a diffusion Monte Carlo method to solve the many-body Schrödinger equation that describes the $X(3872)$ as a $c\bar{c}n\bar{n}$ tetraquark system with quantum numbers $J^{PC} = 1^{++}$. Among other advantages, this approach avoids the usual quark-clustering assumed in any theoretical technique applied to the same problem and, moreover, provides information about the hadron's wave function and structural properties.

The interaction between particles was modeled by the most general and accepted potential, i.e., a pairwise interaction including Coulomb, linear-confining and hyperfine spin-spin terms. There are also Goldstone-boson exchange interactions between light quarks that have been fixed somewhere else reproducing hadron, hadron-hadron and multiquark phenomenology. The chiral contribution to the mass of the $X(3872)$ represent at most 9%, leaving the rest for the general color interaction; note, too, that the chiral potentials are weak and they are not able to produce meson-meson molecular states.

We obtain two $c\bar{c}n\bar{n}$ loosely lying states, with quantum numbers $I^G(J^{PC}) = 0^+(1^{++})$ and $1^-(1^{++})$, whose masses are below the relevant meson-meson thresholds. These states could contribute separately to the observed $X(3872)$ signal, or it may be the result of a coupling between them. According to our results, the two quarks and two antiquarks are arranged as light-meson–heavy-meson molecules of type $\omega J/\psi$ and $\rho J/\psi$, rather than the most extended $D\bar{D}^*$ interpretation. This fact would be the key to make compatible the molecular features of the $X(3872)$ with its decay and production observables that seem to indicate the presence of a $c\bar{c}$ cluster. Finally, its multiplet partners do not show the same behavior, making the $J^P = 1^+$ quantum numbers somewhat special, ideally suited to host molecules.

Finally, analyzing the existence of similar structures in the hidden-bottom sector appears as a natural extension of the method presented herein. Most of the XYZ states have been discovered in the charmonium sector, and not in the bottomonium one, because all the B-factories were originally designed to investigate CP-symmetry violations and thus they had center-of-mass energies that covered 3–5 GeV, which is the typical mass range of charmonium excitations. Experimental facilities, either in operation or planning, have promised the longstanding goal of stuying the bottomonium sector as careful as have been done the charmonium one.

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[2] The space, spin and flavor components of the wave function are omitted without loss of generality.

[3] Within the same formalism, we have calculated the properties of the $|8_{c\bar{c}}\bar{8}_{n\bar{n}}\rangle_{\mathrm{color}}$ state, which would be a color excitation. Its mass is around 150 MeV above the ground state, and its radial distribution functions indicate that it is a compact object.

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