# A Diffusion Monte Carlo technique applied to multiquark systems

M.C. Gordillo
F. De Soto
J. Segovia

Universidad Pablo de Olavide
Sevilla

Goal: Study tetraquarks using a chiral quark model

The interaction between quarks is described by an non-relativistic *effective* Hamiltonian

$$H = \sum_{i=1}^{\text{n-part.}} \left( m_i + \frac{\vec{p}_i^{\,2}}{2m_i} \right) - T_{\text{CM}} + \sum_{j>i=1}^{\text{n-part.}} V(\vec{r}_{ij}),$$

$$V(\vec{r}_{ij}) = V_{CON}(\vec{r}_{ij}) + V_{OGE}(\vec{r}_{ij}) + V_{\chi}(\vec{r}_{ij})$$

For tetraquaks made up only of c and b quarks and their antiparticles

$$V(\vec{r}_{ij}) = V_{\mathrm{OGE}}(\vec{r}_{ij}) + V_{\mathrm{CON}}(\vec{r}_{ij}).$$

$$V_{\mathrm{OGE}}(\vec{r}_{ij}) = \frac{1}{4}\alpha_s(\vec{\lambda}_i \cdot \vec{\lambda}_j)\left[\frac{1}{r_{ij}} - \frac{2\pi}{3m_i m_j}\delta^{(3)}(\vec{r}_{ij})(\vec{\sigma}_i \cdot \vec{\sigma}_j)\right]$$

$\sigma_i$ $\sigma_j$ Pauli matrices (spin)

$$V_{\mathrm{CON}}(\vec{r}_{ij}) = (br_{ij} + \Delta)(\vec{\lambda}_i \cdot \vec{\lambda}_j),$$

$\lambda_i$ $\lambda_j$ Gell-Mann matrices (color)

$$\delta^{(3)}(\vec{r}_{ij}) \to \kappa \frac{e^{-r_{ij}^2/r_0^2}}{\pi^{3/2} r_0^3},$$

Parameters taken from

B. Silvestre-Bragg Few-Body Syst. 20 1 (1996)

For tetraquarks with light quarks (u,d) and/or their antiparticles

$$V_\chi(\vec{r}_{ij}) = V_\sigma(\vec{r}_{ij}) + V_\pi(\vec{r}_{ij}) + V_\eta(\vec{r}_{ij})$$

$$V_\sigma(\vec{r}_{ij}) = -\frac{g_{ch}^2}{4\pi}\frac{\Lambda_\sigma^2}{\Lambda_\sigma^2 - m_\sigma^2} m_\sigma \left[Y(m_\sigma r_{ij}) - \frac{\Lambda_\sigma}{m_\sigma} Y(\Lambda_\sigma r_{ij})\right],$$

$$V_\pi(\vec{r}_{ij}) = \frac{g_{ch}^2}{4\pi}\frac{m_\pi^2}{12 m_i m_j}\frac{\Lambda_\pi^2}{\Lambda_\pi^2 - m_\pi^2} m_\pi \left[Y(m_\pi r_{ij}) - \frac{\Lambda_\pi^3}{m_\pi^3} Y(\Lambda_\pi r_{ij})\right] \times$$

$$\times (\vec{\sigma}_i \cdot \vec{\sigma}_j) \sum^{3} (\lambda_i^a \cdot \lambda_j^a),$$

$$V_\eta(\vec{r}_{ij}) = \frac{g_{ch}^2}{4\pi}\frac{m_\eta^2}{12 m_i m_j}\frac{\Lambda_\eta^2}{\Lambda_\eta^2 - m_\eta^2} m_\eta \left[Y(m_\eta r_{ij}) - \frac{\Lambda_\eta^3}{m_\eta^3} Y(\Lambda_\eta r_{ij})\right] \times$$

$$\times (\vec{\sigma}_i \cdot \vec{\sigma}_j) \left[\cos\theta_p \left(\lambda_i^8 \cdot \lambda_j^8\right) - \sin\theta_p\right],$$

$\sigma_i$ $\sigma_j$ Pauli matrices (spin)

$\lambda_i$ $\lambda_j$ Gell-Mann matrices (flavor)

G. Yang et al PRD 101 014001 (2020)

Effective Hamiltonian → Schrödinger equation

Diffusion Monte Carlo (DMC)

Technique used in many-body condensed matter physics to obtain the ground state (T = 0) of a system of interacting particles

M. H. Kalos, Phys. Rev. A 2 250 (1970)

DMC uses the analogy between the imaginary form of the time-dependent (it ➛ t) Schrödinger equation and a diffusion equation for finding solutions of the time-independent Schrödinger equation

$$-\frac{\partial \Psi_{\alpha'}(\boldsymbol{R},t)}{\partial t} = (H_{\alpha'\alpha} - E_s)\Psi_{\alpha}(\boldsymbol{R},t),$$

$\psi_\alpha$ (R,t) is the exact wavefunction for channel α. We used instead

$f_\alpha(R,t) = \psi(R)\ \ \psi_\alpha(R,t)$

Trial function: Information known a priori

Channel: Each possible spin-color function compatible with the symmetry of the tetraquark

$\psi$(R) is the exact solution of a simplified form of the OGE potential

$$V_{\mathrm{OGE}}(\vec{r}_{ij}) = \frac{1}{4}\alpha_s(\vec{\lambda}_i \cdot \vec{\lambda}_j)\left[\frac{1}{r_{ij}} - \cancel{\frac{2\pi}{3m_i m_j}\delta^{(3)}(\vec{r}_{ij})(\vec{\sigma}_i \cdot \vec{\sigma}_j)}\right]$$

$$\psi(\boldsymbol{R}) = \prod_{i<j}\phi(\vec{r}_{ij}) = \prod_{i<j}\exp(-a_{ij}r_{ij}),$$

1s orbital

$f_\alpha(R,t) = \psi(R) \quad \psi_\alpha(R,t) \Longrightarrow \psi_\alpha(R,t) = f_\alpha(R,t)/\psi(R)$

Substituting that into the Schrödinger equation

$$-\frac{\partial f_{\alpha'}(\boldsymbol{R},t)}{\partial t} = -\frac{1}{2m}\nabla^2_{\boldsymbol{R}} f_{\alpha'}(\boldsymbol{R},t) + \frac{1}{2m}\nabla_{\boldsymbol{R}}[F(\boldsymbol{R})f_{\alpha'}(\boldsymbol{R},t)]$$
$$+[E_L(\boldsymbol{R}) - E_s]f_{\alpha'}(\boldsymbol{R},t) + V_{\alpha'\alpha}(\boldsymbol{R})f_{\alpha}(\boldsymbol{R},t)$$

Potential depending on the channels

$$E_L(\boldsymbol{R}) = \psi(\boldsymbol{R})^{-1} H_0 \psi(\boldsymbol{R}),$$

$$F(\boldsymbol{R}) = 2\psi(\boldsymbol{R})^{-1}\nabla_{\boldsymbol{R}}\psi(\boldsymbol{R})$$

Part of the Hamiltonian independent of the channel

Formal solution for a single channel

$$f_{\alpha'}(\boldsymbol{R}', t+\Delta t) = \sum_{\alpha}\int d\boldsymbol{R}\, G_{\alpha'\alpha}(\boldsymbol{R}', \boldsymbol{R}, \Delta t) f_{\alpha}(\boldsymbol{R}, t).$$

The formal solution for several channels is

$$\mathcal{F}(\boldsymbol{R}, t) = \sum_{\alpha} f_{\alpha}(\boldsymbol{R}, t),$$

Green function
independent of the channel

$$\mathcal{F}(\boldsymbol{R}', t + \Delta t) = \int dR \langle \boldsymbol{R}' | e^{-A\Delta t} | \boldsymbol{R} \rangle \sum_{\alpha' \alpha} e^{-V_{\alpha' \alpha}(\boldsymbol{R})\Delta t} f_{\alpha}(\boldsymbol{R}, t)$$

$$= \int dR \langle \boldsymbol{R}' | e^{-A\Delta t} | \boldsymbol{R} \rangle \omega(\boldsymbol{R}, t) \mathcal{F}(\boldsymbol{R}, t),$$

$$\omega(\boldsymbol{R}, t) = \frac{\sum_{\alpha' \alpha} e^{-V_{\alpha' \alpha}(\boldsymbol{R})\Delta t} f_{\alpha}(\boldsymbol{R}, t)}{\sum_{\alpha} f_{\alpha}(\boldsymbol{R}, t)}.$$

Weight asigned to
each configuration

Quarks are fermions ⟹The wavefunction should be antisymmetric with respect to the interchange of identical quarks

$$
\begin{aligned}
|\bar{3}_{12}3_{34}\rangle = \frac{1}{\sqrt{12}}(&+|rg\bar{r}\,\bar{g}\rangle + |gr\bar{g}\,\bar{r}\rangle - |rg\bar{g}\,\bar{r}\rangle \\
&- |gr\bar{r}\,\bar{g}\rangle + |rb\bar{r}\,\bar{b}\rangle + |br\bar{b}\,\bar{r}\rangle \\
&- |rb\bar{b}\,\bar{r}\rangle - |br\bar{r}\,\bar{b}\rangle + |gb\bar{g}\,\bar{b}\rangle \\
&+ |bg\bar{b}\,\bar{g}\rangle - |gb\bar{b}\,\bar{g}\rangle - |bg\bar{g}\,\bar{b}\rangle),
\end{aligned}
$$

The color functions are the colorless eigenvectors of $F^2 = (\sum \lambda_i /2)^2$

Antisymmetric with respect to the interchange $1 \leftrightarrow 2$ and $3 \leftrightarrow 4$

$$
\begin{aligned}
|6_{12}\bar{6}_{34}\rangle = \frac{1}{\sqrt{6}}[&+|rr\bar{r}\,\bar{r}\rangle + |gg\bar{g}\,\bar{g}\rangle + |bb\bar{b}\,\bar{b}\rangle \\
&+ \frac{1}{2}(+|rg\bar{r}\,\bar{g}\rangle + |gr\bar{g}\,\bar{r}\rangle + |rg\bar{g}\,\bar{r}\rangle \\
&+ |gr\bar{r}\,\bar{g}\rangle + |rb\bar{r}\,\bar{b}\rangle + |br\bar{b}\,\bar{r}\rangle \\
&+ |rb\bar{b}\,\bar{r}\rangle + |br\bar{r}\,\bar{b}\rangle + |gb\bar{g}\,\bar{b}\rangle \\
&+ |bg\bar{b}\,\bar{g}\rangle + |gb\bar{b}\,\bar{g}\rangle + |bg\bar{g}\,\bar{b}\rangle)],
\end{aligned}
$$

Symmetric with respect to the interchange $1 \leftrightarrow 2$ and $3 \leftrightarrow 4$

The spin functions are the eigenvectors of $S^2 = (\sum \sigma_i /2)^2$ for a given value of the total spin of the tetraquark (S= 0, 1,2)

S = 0

$$|\chi_{S=0,S_z=0}\rangle_{SS} = \frac{1}{\sqrt{12}}(+2|\downarrow\downarrow\uparrow\uparrow\rangle + 2|\uparrow\uparrow\downarrow\downarrow\rangle - |\downarrow\uparrow\uparrow\downarrow\rangle - |\uparrow\downarrow\downarrow\uparrow\rangle + |\downarrow\uparrow\downarrow\uparrow\rangle - |\uparrow\downarrow\uparrow\downarrow\rangle),$$

Symmetric with respect to the interchange $1 \longleftrightarrow 2$ and $3 \longleftrightarrow 4$

$$|\chi_{S=0,S_z=0}\rangle_{AA} = \frac{1}{2}(-|\downarrow\uparrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\downarrow\rangle - |\uparrow\downarrow\downarrow\uparrow\rangle + |\uparrow\downarrow\uparrow\downarrow\rangle).$$

Antisymmetric with respect to the interchange $1 \longleftrightarrow 2$ and $3 \longleftrightarrow 4$

$f_\alpha(R,t)$ is not an analytical function but a set of *walkers*

Set of coordinates of the quarks and the coefficients of the different channels, $c_\alpha$. They evolve in imaginary time according to a diffusion process that depends on the particular $\psi(R)$ we have chosen

That diffusion process is directed to the zones of the phase space where $\psi(R)$ is larger $\Longrightarrow$ importance sampling

# Examples of functions with the right symmetry

| | | | |
|---|---|---|---|
| $cc\bar{c}\bar{c}, bb\bar{b}\bar{b}$ | | | |
| $cc\bar{b}\bar{b}$ $(bb\bar{c}\bar{c})$ | $0^{+(+)}$ | $\lvert\chi_{S=0}\rangle_{SS} \otimes \lvert\bar{3}_c 3_c\rangle_{AA}$ | $\lvert\chi_{S=0}\rangle_{AA} \otimes \lvert 6_c\bar{6}_c\rangle_{SS}$ |
| | $1^{+(-)}$ | $\lvert\chi_{S=1}\rangle_{SS} \otimes \lvert\bar{3}_c 3_c\rangle_{AA}$ | |
| | $2^{+(+)}$ | $\lvert\chi_{S=2}\rangle_{SS} \otimes \lvert\bar{3}_c 3_c\rangle_{AA}$ | |

Only two antisymmetric functions under the interchange of identical quarks (1⟷2 and 3 ⟷ 4) out of four possible

$$X_{\text{spin-color}} = c_1\, \lvert\chi_{S=0}\rangle_{SS} \otimes \lvert\bar{3}_c 3_c\rangle_{AA} + c_2\, \lvert\chi_{S=0}\rangle_{AA} \otimes \lvert 6_c\bar{6}_c\rangle_{SS}$$

The DMC algorithm provides both energies (masses) and structural information (distances between particles and probability distributions)

It is NOT variational in nature $\Longrightarrow$ It is able to correct the initial approximation (trial function) to give the exact ground state of the tetraquark by including all the possible correlations between quarks

Our initial approximation does not contain any particular grouping of quarks nor any other limitation beyond the derived from the Pauli principle

$$\psi(\boldsymbol{R}) = \prod_{i<j} \phi(\vec{r}_{ij}) = \prod_{i<j} \exp(-a_{ij} r_{ij}),$$

$$X_{\text{spin-color}} = c_1 \, |\chi_{S=0}\rangle_{SS} \otimes |\bar{3}_c 3_c\rangle_{AA} + c_2 \, |\chi_{S=0}\rangle_{AA} \otimes |6_c \bar{6}_c\rangle_{SS}$$

# Proof of concept: mass of heavy mesons…

| | $n^{2S+1}L_J$ | $J^{PC}$ | DMC | VAR [54] | EXP [13] |
|---|---|---|---|---|---|
| $\eta_c$ | $1^1S_0$ | $0^{-+}$ | 3005 | 3006.6 | $2983.9 \pm 0.5$ |
| $J/\psi$ | $1^3S_1$ | $1^{--}$ | 3101 | 3102.1 | $3096.900 \pm 0.006$ |
| $B_c$ | $1^1S_0$ | $0^{-+}$ | 6292 | 6293.5 | $6274.9 \pm 0.8$ |
| $B_c^*$ | $1^3S_1$ | $1^{--}$ | 6343 | $\cdots$ | $\cdots$ |
| $\eta_b$ | $1^1S_0$ | $0^{-+}$ | 9424 | 9427.9 | $9398.7 \pm 2.0$ |
| $\Upsilon(1S)$ | $1^3S_1$ | $1^{--}$ | 9462 | 9470.4 | $9460.30 \pm 0.26$ |

[54] G.J. Yang et al PRD 100 096013 (2018)
[13] PDG PRD 98 030001 (2018)

# … and of heavy baryons

| Baryon | $^{2S+1}L_J$ | $J^P$ | DMC | Ref. [59] |
|---|---|---|---|---|
| $\Omega_{ccc}^{++}$ | $^4S_{3/2}$ | $3/2^+$ | 4798 | 4799 |
| $\Omega_{ccb}^{+}$ | $^2S_{1/2}$ | $1/2^+$ | 8018 | 8019 |
| $\Omega_{cbb}^{0}$ | $^2S_{1/2}$ | $1/2^+$ | 11215 | 11217 |
| $\Omega_{bbb}^{-}$ | $^4S_{3/2}$ | $3/2^+$ | 14398 | 14398 |

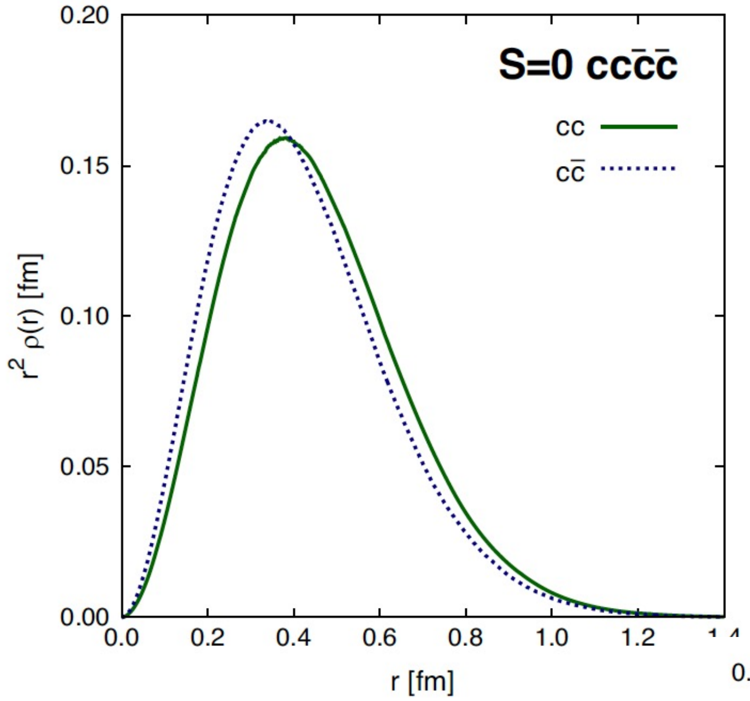
[59] B. Silvestre-Brac, Few-Body Syst. 20, 1 (1996).

cc $\overline{cc}$

Masses obtained with the same effective potential

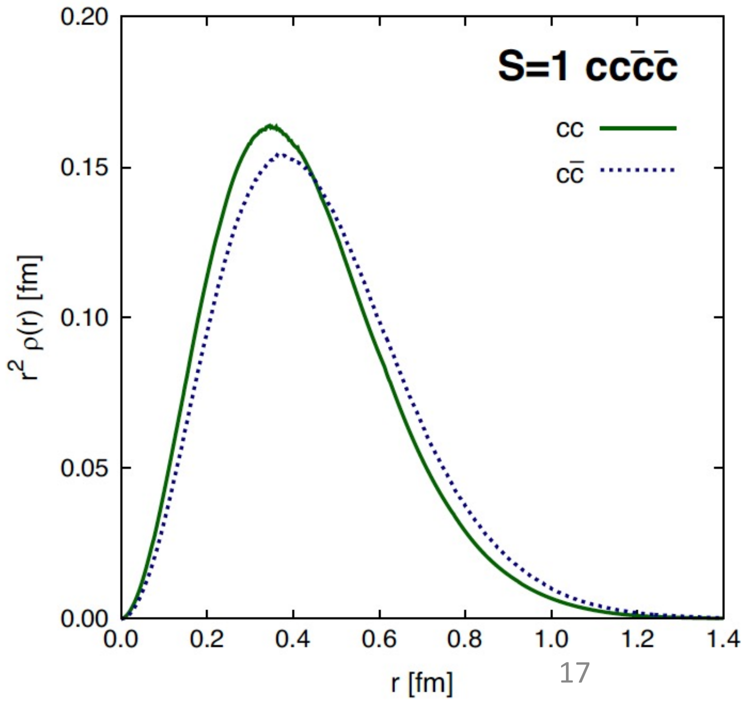
| $J^{PC}$ | DMC | VAR [54] |
|---|---|---|
| $0^{++}$ | 6351 | 6371 |
| $1^{+-}$ | 6441 | 6450 |
| $2^{++}$ | 6471 | 6479 |

The inclusion of correlations decreases the mass




Meson-meson

Diquark-antidiquark




M.C. Gordillo et al
PRD 102 114007 (2020)

$bb\overline{bb}$

| $J^{PC}$ | DMC | VAR [54] |
|---|---|---|
| $0^{++}$ | 19 199 | 19 243 |
| $1^{+-}$ | 19 276 | 19 311 |
| $2^{++}$ | 19 289 | 19 325 |

$cb\overline{cb}$

| $J^{PC}$ | DMC | [33] | [35] | [36] |
|---|---|---|---|---|
| $0^{++}$ | 12 534 | 12 854 | 12 359 | 13 396 |
| $1^{+-}$ | 12 510 | 12 881 | 12 424 | 13 478 |
| $1^{++}$ | 12 569 | 12 933 | 12 485 | 13 510 |
| $2^{++}$ | 12 582 | 12 933 | 12 566 | 13 590 |

$cc\overline{cb}$ $bb\overline{bc}$

| $J^{P}$ | DMC | [33] | [36] | DMC | [33] | [36] |
|---|---|---|---|---|---|---|
| $0^{+}$ | 9615 | 9715 | 10 144 | 16 040 | 16 141 | 16 823 |
| $1^{+}$ | 9610 | 9727 | 10 174 | 16 013 | 16 148 | 16 840 |
| $2^{+}$ | 9719 | 9768 | 10 273 | 16 129 | 16 176 | 16 917 |

[54] G.J. Yang et al PRD 100 096013 (2018). [35] A. Berezhnoy et al, PRD 86, 034004 (2012).
[33] M.-S. Liu et al PRD 100, 016006 (2019) [36] L. Reinders et al , Phys. Rep. 127, 1 (1985).

## Application to X(3872)

Mass at the $D^0 \bar{D}^{0*}$ threshold

Quantum numbers $J^{PC} = 1^{++}$

Decays at the same ratio into
$\rho J/\psi$ and $\omega$ $J/\psi$

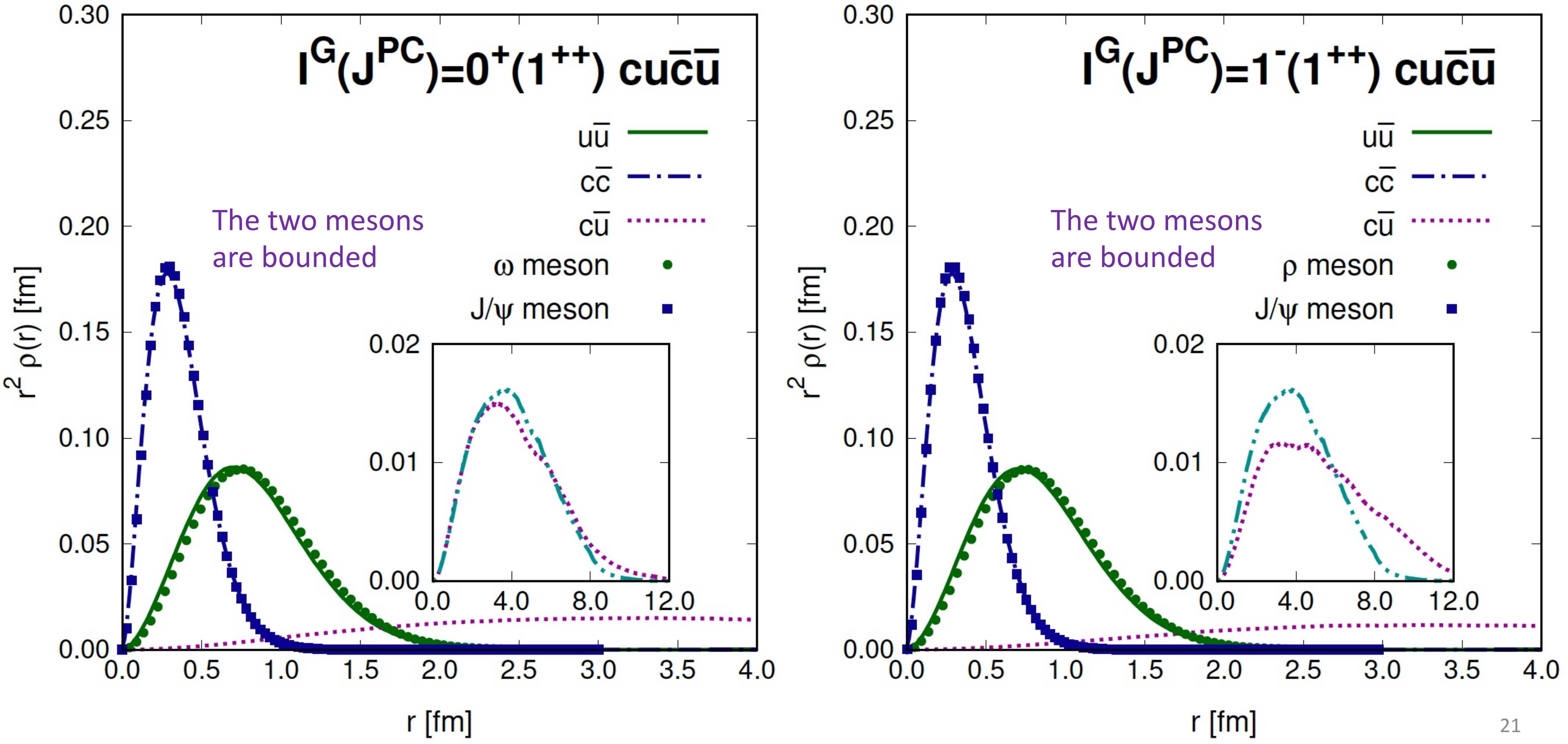
Radiative decays into $\Upsilon J/\psi$ and $\Upsilon\psi(2S) \Longrightarrow$
at least partial $c\bar{c}$ component

Experimental data

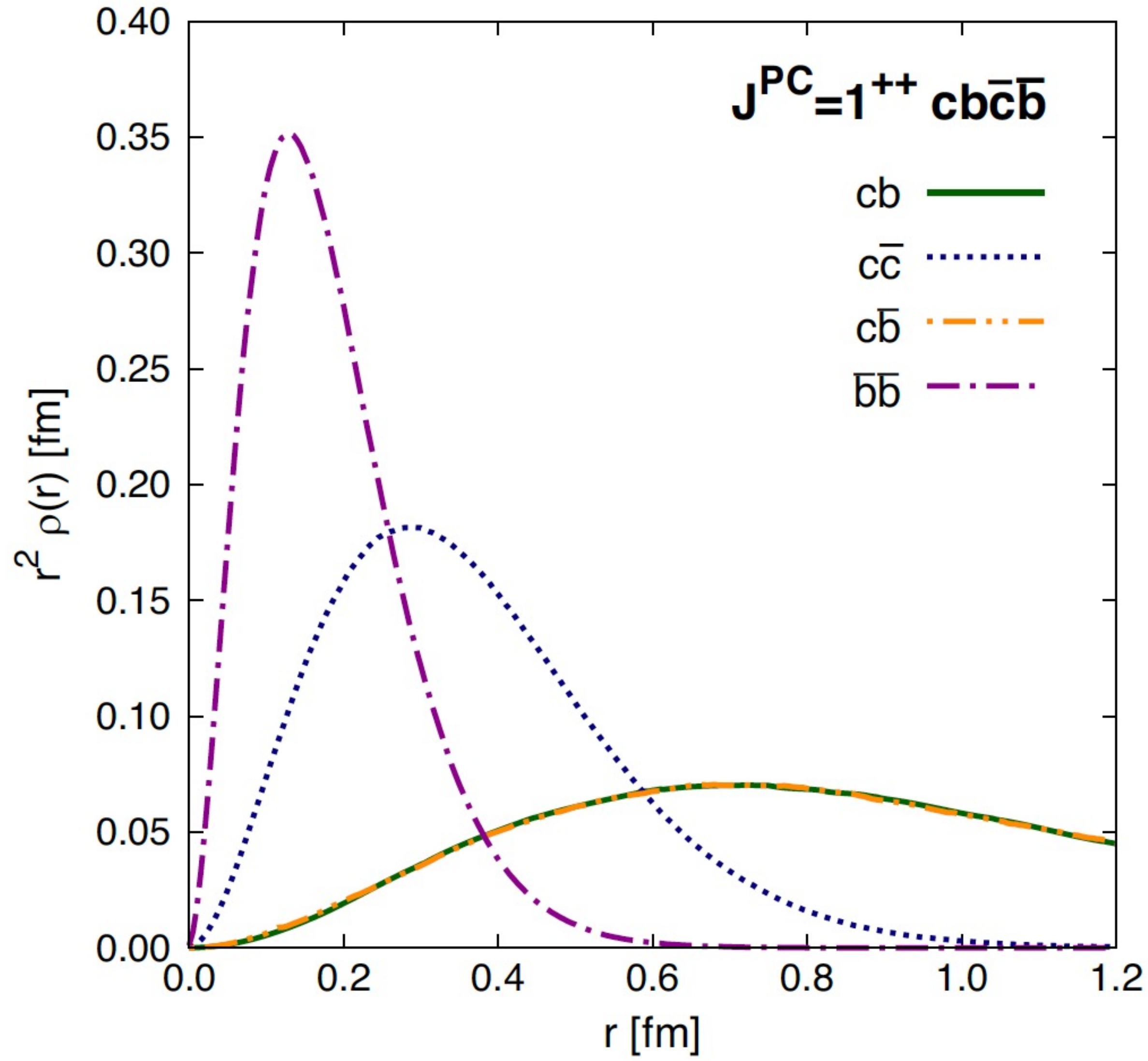
# Description of X(3872) as a $c\bar{c}\, n\bar{n}$ tetraquark (n= u,d) $\Longrightarrow$ DMC calculation

| | $M_e$ [10] | $M_f$ | $M_\chi$ | |
|---|---|---|---|---|
| $\rho$ | 775 | 770 | 770 | |
| $\omega$ | 783 | 769 | 770 | |
| $D$ | 1868 | 1863 | 1863 | 3877 MeV |
| $D^*$ | 2009 | 2016 | 2016 | 3879 MeV |
| $J/\psi$ | 3097 | 3101 | 3101 | |
| $c\bar{c}u\bar{u}$ $(I=0)$ | - | 3834 | 3874 | Lower mass |
| $c\bar{c}u\bar{u}$ $(I=1)$ | - | 3842 | 3874 | |
| | Experiment | Full calculation | "Flavorless" data | |

# Structure of the X(3872) as a tetraquark ⟹ ω + J/ψ or ρ + J/ψ



A similar pairing appears also in all-heavy tetraquarks with similar quantum numbers




$$|X(3872)\rangle_{\rm color} = c_1\,|\bar{3}_{nc}3_{\bar{n}\bar{c}}\rangle_{\rm color} + c_2\,|6_{nc}\bar{6}_{\bar{n}\bar{c}}\rangle_{\rm color} \Rightarrow |X(3872)\rangle_{\rm color} \approx |1_{c\bar{c}}\bar{1}_{n\bar{n}}\rangle_{\rm color}$$

# Sumarizing …

We have used the diffusion Monte Carlo technique to describe tetraquarks in the chiral quark model considering all the couplings between channels

In the X(3872) case, it appears that a meson-meson molecular configuration is preferred but, contrary to the usual assumption of a $D^0 \overline{D^0}{}^*$ molecule our formalism produces $\omega + J/\psi$ (I=0) or $\rho + J/\psi$ (I=1) clusters as the most stable ones

The DMC technique is scalable and it is expected to work for larger quark clusters (penta- and hexaquarks)

$D^0\overline{D^0}{}^*$