Femtoscopic study of the proton-deuteron interaction

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In recent studies of the proton-deuteron femtoscopic correlation function, the Lednický approximation is employed to describe the wave function of the two-body system, but the results deviate strongly from experimental data of the ALICE collaboration, and suggest the need for a full three-body study. Considering these challenges, an alternative approach is proposed by solving the proper wave function of the two-body Schrödinger equation, using a numerical program following the Numerov algorithm. This simple model describes the ALICE data reasonably well.

I. INTRODUCTION

As its name suggests, femtoscopy is the discipline that explores, at femtometer distances, the behavior of subatomic particles and the forces that govern their interactions [1]. Particle accelerators are used to collide them at high energies, and highly sophisticated detectors are employed to detect the particles generated from these collisions. Projects such as ALICE, an international collaboration at CERN's LHC, and STAR, from RHIC at BNL, focus on the study of ion collisions and, recently, proton-deuteron pairs have been measured [2]. The femtoscopic analysis of the data involves calculating the wave function of the system, and approximation methods such as the Lednický model [3] for two-body type wave-functions, have been employed. However, these wave functions and their corresponding correlation functions differ substantially from the experimental data of the ALICE collaboration (see the Appendix for details). Due to these results, it was advocated that a full three-body description of the proton-deuteron scattering problem [4], which accounts for the intrinsic structure of the deuteron, was strictly necessary. The purpose of this work is to explore whether a two-body description of proton-deuteron scattering, not relying on the wave function of the Lednický model, can still provide a reasonable account of the experimental correlation function. To this end, a proton-deuteron two-body wave function will be obtained by solving the Schrodinger equation with appropiate interaction potentials. To address this problem, a computational procedure has been developed and implemented in a Fortran code that determines numerically the two-body wave function, from which the femtoscopic correlation function is extracted and compared with the recent experimental data of the ALICE collaboration.

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II. FORMALISM

A. Wave function of the proton-deuteron pair

We start our methodology by solving the two-body time-independent Schrödinger equation for a Woods-Saxon (WS) potential ($V_{WS}(r)$),

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi(\vec{r}) + V_{WS}(r)\psi(\vec{r}) = E\psi(\vec{r}) \ , \qquad (1)$$

where μ is the reduced mass and $E = \hbar^2 k^2/2\mu$ is the total energy of the system in the center of mass frame. The WS potential represents the strong interaction between a proton and a deuteron,

$$V_{WS}(r) = -\frac{V_0}{1+\mathrm{e}^{(r-R)/a}} \ , \qquad (2)$$

where V_0, a, and R are constants given in Table I and taken from Ref. [5].

	V_0 (MeV)	R (fm)	a (fm)
$J = 1/2$	29.754	2.826	1.187
$J = 3/2$	18.115	2.837	0.9655

TABLE I: Values from Ref. [5] for the potential depth, V_0, the size, R, and the surface thickness parameter, a, of WS-type proton-deuteron potentials, fitted to reproduce the experimental phase-shifts in both total spin values $J = 1/2$ and $J = 3/2$.

Exploiting the rotational invariance of $V_{WS}(r)$, we can propose a separable wave function solution in the following form,

$$\psi(r,\theta,\phi,k) = \sum_{l,m} \Phi_l(r,k) Y_l^m(\theta,\phi) \ , \qquad (3)$$

where $\Phi_l(r,k)$ is the radial wave function and $Y_l^m(\theta,\phi)$ represents the spherical harmonics. By introducing the reduced wave function $u_l(r,k)$ as $\Phi_l(r,k) = u_l(r,k)/r$, we obtain the following equation that only depends on the radial coordinate,

$$\left(\frac{d^2}{dr^2} + k^2 - U(r) - \frac{l(l+1)}{r^2}\right) u_l(r,k) = 0 \qquad (4)$$

where $U(r) = 2\mu V_{WS}(r)/\hbar^2$, and l is the orbital quantum number. From now on, we will use natural units, namely $\hbar = 1$ and $c = 1$.

The reduced radial wave function has been numerically solved using the Numerov algorithm [6], a finite difference method that calculates the shape of the wave function by integrating step by step along a grid. For bound states, for which the wave function is normalizable, a matching point $r = R_m$ outside of the potential was chosen. A wave function, $u_l^{\text{left}}(r)$, was computed from $r = 0$ until $r = R_m$; and another wave function, $u_l^{\text{right}}(r)$, was computed in the reverse direction from a large value of r, say $r = 10R_m$, until $r = R_m$.

The bound state is determined by finding the binding energy $E_0 < 0$ for which the function $u_l(r)$ and its derivative $u_l'(r)$ are continuous at R_m. Since we do not know this energy at first, a bisection method is applied starting with $E = 0$ and $E = \min(V_{WS})$.

For continuum states, with positive energies, the numerical solution is evolved beyond the matching point R_m, where the Woods-Saxon potential will be close to zero. In this case, one fixes the value of $E > 0$ and the Numerov algorithm is numerically performed by increasing r. One does not require $u_l^{\text{right}}(r)$. Asymptotically, the wave function will almost resemble that of a free particle and it can be expressed in terms of spherical Bessel (j_l) and Neumann (n_l) functions as follows [7]:

$$u_l(r,k) = re^{i\delta_l(k)}[\cos\delta_l j_l(kr) - \sin\delta_l n_l(kr)] \ , \quad (5)$$

where $\delta_l(k)$ is a phase shift. For $\delta_l(k) = 0$, the behavior is that of a particle without any interaction. To extract the value of the phase-shift we define a dimensionless logarithmic derivative, incorporating the factor r, in the following manner,

$$\beta_l(k) = \left[r\frac{u_l'(r,k)}{u_l(r,k)}\right]_{r=R_\infty} \ , \quad (6)$$

which is applied at a sufficiently distant point R_∞ in order to neglect the effects of the strong potential. We have chosen it to be 9 times the matching point, $R_\infty = 9R_m$. By numerically computing this logarithmic derivative with our solution, and making use of the asymptotic form in Eq. (5), we can ultimately find the phase shift from:

$$\tan\delta_l(k) = \frac{kR_\infty j_l'(kR_\infty) - (\beta_l - 1)j_l(kR_\infty)}{kR_\infty n_l'(kR_\infty) - (\beta_l - 1)n_l(kR_\infty)} \ . \quad (7)$$

Finally, once the phase shift has been obtained, we can fix the overall normalization constant of our wave function by matching with the form in Eq. (5) at $r = R_\infty$.

Since both proton and deuteron carry electrical charge, we need to account for electromagnetic effects. If we add the Coulomb interaction to the Woods-Saxon potential, the formalism needs to be changed. The numerical algorithm to find the wave function only requires the replacement

$$V_{WS}(r) \to V_{WS}(r) + \frac{\alpha}{r} \ , \quad (8)$$

with $\alpha = 1/137$. At $r > R_m$, the Coulomb potential still has significant effects, whereas the term corresponding to the Woods-Saxon effect practically disappears. Therefore, following the previous reasoning, a particle that has been under the influence of a Woods-Saxon potential with Coulomb effects will, at long distances, behaves like a particle with only Coulomb effects but with an extra phase shift relative to a non-interacting particle with the strong force. Thus, the function $u_l^{\text{C+S}}(r,k)$ for asymptotic long distances can be expressed as [8]

$$u_l^{\text{C+S}}(r,k) = k^{-1}e^{i\Delta_l}\left[\cos\hat{\delta}_l F_l(\gamma;kr) - \sin\hat{\delta}_l G_l(\gamma;kr)\right] \ , \quad (9)$$

where $\gamma = \mu\alpha/k$, F_l and G_l are, respectively, the regular and irregular Coulomb wave functions in [9] and $\Delta_l = \sigma_l + \hat{\delta}_l$ is a global phase-shift that contains the so-called Coulomb phase shift, $\sigma_l = \arg\Gamma(1+l+i\gamma)$, and a phase shift, $\hat{\delta}_l$, that represents the effect of the strong interaction, not equal to the δ_l defined before for a pure strong interaction case.

Continuing with the analogy of the strong interaction case, we can calculate the dimensionless logarithmic derivative of $u_l^{\text{C+S}}(r,k)$, exactly as defined in Eq. (6), which has been numerically computed using the Numerov algorithm. Comparing with the asymptotic expression of Eq. (9), one can finally write the phase shift in this case as

$$\tan\hat{\delta}_l(k) = \frac{kR_\infty F_l'(\gamma;kR_\infty) - \beta_l F_l(\gamma;kR_\infty)}{kR_\infty G_l'(\gamma;kR_\infty) - \beta_l G_l(\gamma;kR_\infty)} \quad (10)$$

with $R_\infty = 9R_m$. Note also that we can normalize the wave function by matching the numerically obtained wave function with the expression of Eq. (9) at the radial distance $r = R_\infty$.

B. Femtoscopy correlation function

Once we have solved the Schrödinger equation, and we have numerically calculated and properly normalized the wave function, we proceed with the femtoscopic study of the proton-deuteron system. We define the femtoscopy correlation function as in Ref [1]:

$$C(k) = \int S(r)\,|\Phi(r,k)|^2\,d^3r \ , \quad (11)$$

where the first term of the integrand describes the source function that emits the particles, and the second term is the two-body wave function. The experimental source function is chosen by a Gaussian profile that depends only on the relative distance r:

$$S(r) = \left(4\pi r_0^2\right)^{-3/2}\exp\left(-\frac{r^2}{4r_0^2}\right) \ , \quad (12)$$

where r_0 is the radius parameter that defines the size of the source.

We first consider the strong interaction case only. Since we are interested in the scattering at low-energies, the modified wave function can be approximated as a plane wave with only the s-wave term modified as follows,

$$\Phi^S(r,k) = e^{i\vec{k}\vec{r}} - j_0(kr) + \Phi_0^S(r,k) \ , \tag{13}$$

where $\Phi_0^S(r,k)$ is the wave function containing the strong interaction effects in s-wave. Replacing the wave function appearing in the definition of the correlation function by the above decomposition we obtain

$$C(k) = 1 + \int S(r) \left[\left| \frac{u_0^S(r,k)}{r} \right|^2 - j_0^2(kr) \right] d^3r \ . \tag{14}$$

where $u_0^S(r,k)$ is the reduced radial s-wave function that has been numerically solved using the method explained in the previous section.

We now derive the expression of the correlation function when Coulomb effects are also included. Following the previous methodology, the wave function with strong interaction plus Coulomb effects, $\Phi^{\mathrm{C+S}}$, is obtained from the asymptotic complete Coulomb wave function, Φ_f^C, with the corresponding s-wave component replaced by that containing the effect of the strong interaction as

$$\Phi^{\mathrm{C+S}}(k;r,z) = \Phi_f^C(k;r,z) - \Phi_{0f}^C(kr) + \Phi_0^{\mathrm{C+S}}(k;r) \ , \tag{15}$$

where $z = r\cos\theta$, with θ being the relative angle between $\vec{r}$ and $\vec{k}$. The complete Coulomb wave function including all partial waves is given by [8]

$$\Phi_f^C(k;r,z) = e^{-\pi\gamma/2}\Gamma(1+i\gamma)e^{ikz}{}_1F_1(-i\gamma;1;ik(r-z)) \ , \tag{16}$$

with $\Gamma(z)$ being the Euler's gamma function and ${}_1F_1(a,b;z)$ the confluent hypergeometrical function or Kummers function. The s-wave projection of the Coulomb wave function is given by [8],

$$\Phi_{0f}^C(kr) = (kr)^{-1}e^{i\sigma_0}F_0(\gamma;kr) \ , \tag{17}$$

as can also be checked from Eq. (9) after setting $l = 0$, $\hat{\delta}_0 = 0$ and taking into account that $\Phi_{0f} = u_0/r$.

Expanding the second term of the correlation function integral in a similar way to the previous case leads to the following expression for the correlation function that considers the effect of both the strong and the electromagnetic interactions:

$$C(k) = \int S(r) \left|\Phi_f^C(k;r,z)\right|^2 d^3r + \int 4\pi r^2 S(r) \left[\left| \frac{u_0^{C+S}(r,k)}{r} \right|^2 - \left|\Phi_{0f}^C(kr)\right|^2 \right] dr \ , \tag{18}$$

where $u_0^{\mathrm{C+S}}(r,k)$ represents the computed reduced radial s-wave function, obtained through the numerical solution method detailed in the preceding section.

III. NUMERICAL RESULTS

The results presented here have been obtained from a Fortran code that incorporates i) the Numerov method to obtain the normalized radial wave function, ii) an evaluation of phase shifts and iii) the computation of the correlation function, for different types of potentials and spin values. The code has been entirely developed for this particular study. An analysis of the results allows us to draw meaningful conclusions about the present study.

A. Wave functions and scattering phase-shifts

To conduct the femtoscopy study of the system, we first need the wave functions to apply them. We will begin by representing the potentials for $l = 0$ using the data from Table I.

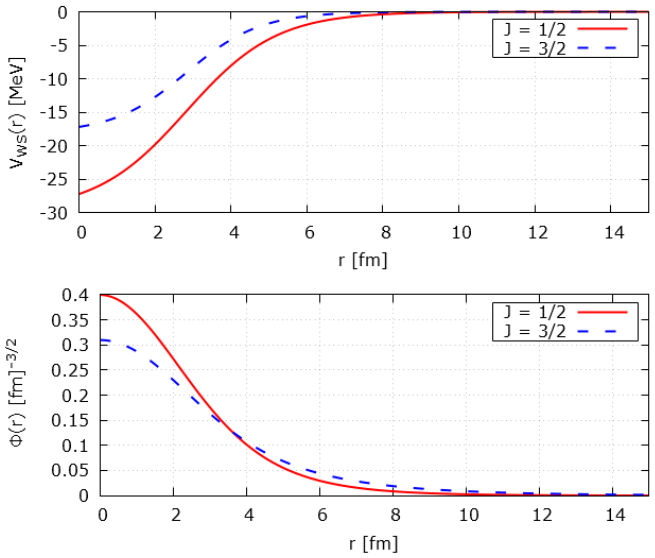

FIG. 1: Top: Strong interaction potentials with Woods-Saxon form. Bottom: s-wave functions of bound states for both spin values.

To numerically solve the Schrödinger equation, the Numerov algorithm was implemented as explained in the previous section to calculate the bound states. For the normalization of these wave functions, only a constant that makes satisfy the normalization integral $4\pi \int dr[u_0^S(r,k)]^2 = 1$ is required. The wave functions of the bound states correspond to the energies of $E(J = 1/2) = -7.780$ MeV, which coincides with the binding energy of the ^{3}He nucleus, and $E(J = 3/2) = -2.539$ MeV. In Fig. 1 it can be observed that for $J = 1/2$, the depth of the potential well is greater, and consequently, its wave function is more pronounced at the origin.

We move on to the continuous spectrum of positive energy states, $E > 0$. To solve these wave functions, the method explained earlier for positive energies was followed. These wave functions have been normalized

by finding their respective phase shifts and performing a matching. Subsequently, we have figures representing the phase shift for each total spin case in Fig. 2, as functions of the kinetic energy of the incident proton in the lab frame, which is given by $T_p = E(m_p + m_d)/m_d$, with m_p and m_d being the proton and deuteron mass, respectively.

As seen in Fig. 2, the numerically computed phase shifts closely approximates the behavior of experimental data extracted from Ref. [10]. With these phase shifts, the wave function for only strong interactions can be normalized.

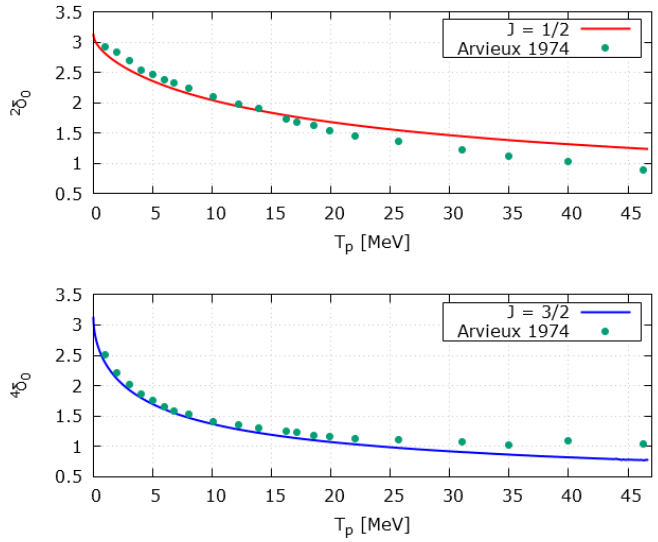

FIG. 2: Values of the s-wave phase shifts, $^2\delta_0$ and $^4\delta_0$, as functions of the kinetic energy of the incident proton, compared with the experimental data from Ref. [10].

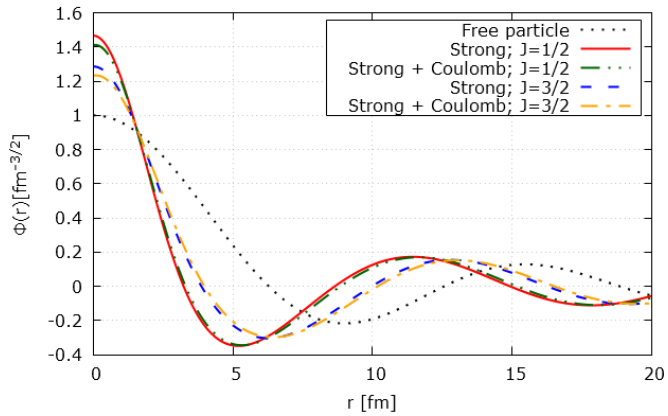

FIG. 3: Wave functions for $k = 0.5$ fm^{-1} of a free particle, a particle with only strong interaction, and a particle with strong and Coulomb interactions for total spin $J = \frac{1}{2}, \frac{3}{2}$.

Adding the Coulomb potential to the strong force, we follow the same procedure to numerically calculate the wave functions, and for their normalization, we use the phase shifts $\hat{\delta}_l(k)$ for the matching. Fig. 3 provides a visual summary of everything we have analyzed so far. We can observe the effect of the strong attractive potential on the wave functions (red and dashed-blue lines), which, compared to that of a free particle (dotted black line), is pulled in, making it more intense at the origin and producing a repulsive phase-shift. If we compare these strong wave functions with the corresponding S+C wave functions (dash-doubly-dotted green and dash-dotted yellow lines), what include also the effect of the repulsive Coulomb force, we can observe a mild decrease of the wave function at the origin and a small shift to higher distances.

B. Femtoscopy correlation functions

Once we have reached this point, we can put into practice what has been derived from the femtoscopy formalism and represent the numerical results compared with the experimental data. Starting from Eq. (9), normalized with the corresponding phase-shift solved with Eq. (10), we represent the obtained correlation functions for different spin cases in Fig. 4.

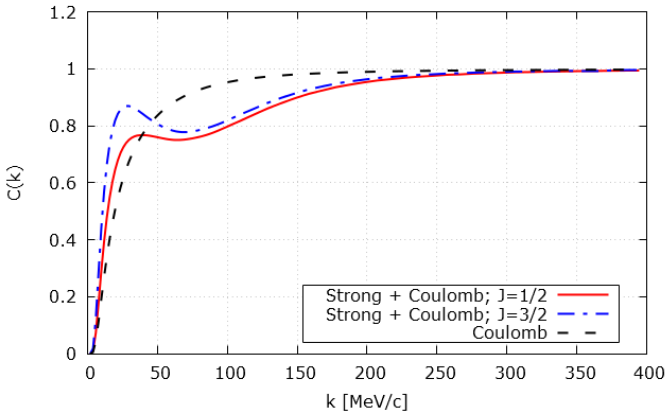

FIG. 4: Correlation functions for a source radius parameter, $r_0 = 1.25$ fm, for both spin values with Coulomb and strong interactions incorporated, and only Coulomb, for comparison.

The lines in the graph in Fig. 4 need to be combined to extract the total correlation function, taking a spin-weighted average. Note that for $J = 1/2$, there are two possible states, $[1/2; -1/2]$, and for $J = 3/2$, there are four states, namely $[3/2; 1/2; -1/2; -3/2]$. Therefore,

$$C(k) = \frac{2\,{}^2C(k) + 4\,{}^4C(k)}{6} \,. \tag{19}$$

The Coulomb-only correlation function is < 1, indicating repulsion. The strong attractive component, when the strong interaction is applied, causes it to grow more rapidly. Following this procedure for different values of the source radius, we arrive at the results in Fig. 5. We can see that the numerically obtained results closely

match the experimental data. With a simple model like the one used in this study, we have successfully replicated a behavior very similar to the experimental findings. It is notable that for larger values of r_0, the numerical results converge more closely to the experimental data, avoiding the first peak. This convergence becomes more pronounced for smaller r_0, suggesting that in the source, there are more pairs with a small relative distance. Consequently, the interaction with the strong force becomes more significant. Therefore, realistic values for r_0 corresponding to the proton-deuteron collision would be $r_0 = 1.5, 1.75$ and 2 fm.

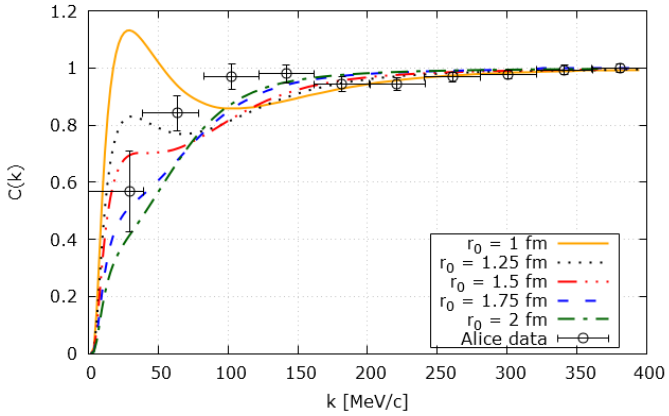

FIG. 5: Correlation functions for different source radius parameter values with Coulomb and strong interactions compared with the experimental data extracted from Ref. [1].

IV. CONCLUSIONS

We have developed a Fortran program, based on the Numerov's algorithm, to solve the Schrödinger equation of a two-body problem employing a simple interaction, the Wood-Saxon plus the Coulomb potential, to determine the corresponding wave function. We have aimed at investigating if the correlation function obtained with this wave function is capable of reproducing the recently available experimental results.

Using our numerically solved wave function, we have found accurate expressions for the phase shifts and the femtoscopy correlation function. This has allowed us to have a reasonably good theoretical description for the experimental data, especially considering the simplicity of the model. Obviously, as we can see in Ref. [4], the interaction described by a three-body problem will be more realistic. However, our calculation with a two-body system can still be improved further with a more sophisticated calculation that takes into account higher partial waves or by adding new interactions to the potential, such as spin-spin or isospin-dependent interactions.

In previous works, Coulomb and strong interactions were implemented into the correlation function using the Lednický model [3], which yielded results incompatible with experimental data [2] (see the discussion and figure in the Appendix).

Due to the results obtained from the approximation with the Lednický model, it was believed that an internal description of the deuteron was necessary, transforming this problem into a three-body calculation. This work demonstrates that with a realistic two-body wave function, obtained from the solution of the Schrödinger equation with *pd* potentials that reasonably describe the phase shifts, we find a correlation function that closely resembles the experimentally measured one.

Acknowledgments

I wish to express my gratitude to my mentors, who have provided me with the opportunity to immerse myself in the world of physics research. The chance to stay abreast of developments in nuclear physics has been an enriching experience, unveiling a deep passion for this branch of physics, which I consider valuable for my future development. Likewise, I want to extend my gratitude to my family, friends, and my partner for their unwavering support. Their constant motivation has been pivotal, inspiring me each day to pursue the goals that I truly desire.

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V. APPENDIX: LEDNICKÝ MODEL FOR PROTON-DEUTERON

The so-called Lednický approximation [3] to the correlation function is obtained when one inserts into Eq. (11) the asymptotic form of the wave function. A further assumption is involved, consisting in replacing the scattering amplitude with total spin J, $f^J(k)$, which multiplies the scattered spherical component of the wave function, by its so-called low-energy expansion expression,

$$f^J(k) = \left(\frac{1}{a_0^J} + \frac{1}{2}d_0^J k^2 - ik\right)^{-1}, \tag{20}$$

where a_0^J is the scattering length and d_0^J is the effective range parameter of the interaction in the spin channel J.

As already said, in this approximation the interaction wave function is the asymptotic one, even close to the interacting potential, what is not fully correct. However the final expression for $C_{\mathrm{LL}}(k)$ is analytic. For example, the expression for the correlation function (without Coulomb effects, for simplicity) is [1]

$$C_{\mathrm{LL}}(k) = 1 + \sum_{J=\{\frac{1}{2},\frac{3}{2}\}} \left[\frac{1}{2}\left|\frac{f^J(k)}{r_0}\right|^2 \left(1 - \frac{a_0^J}{2\sqrt{\pi}r_0}\right) + \frac{2\mathrm{Re}\ f^J(k)}{\sqrt{\pi}r_0}F_1(2kr_0) - \frac{\mathrm{Im}\ f^J(k)}{r_0}F_2(2kr_0)\right], \tag{21}$$

where $F_1(x)$ and $F_2(x)$ are analytical functions that result from the Gaussian parametrization of the source function.

There exists another expression valid for the case with both strong and Coulomb effects. Since it is more complicated, we reproduce here the case with strong interaction only.

The ALICE collaboration has used this model to predict the correlation function of a proton-deuteron pair using a source radius parameter of $r_0 = 1.08$ fm, and several strong interaction potentials; among them, the one from Arvieux [10], the same that we use in this work.

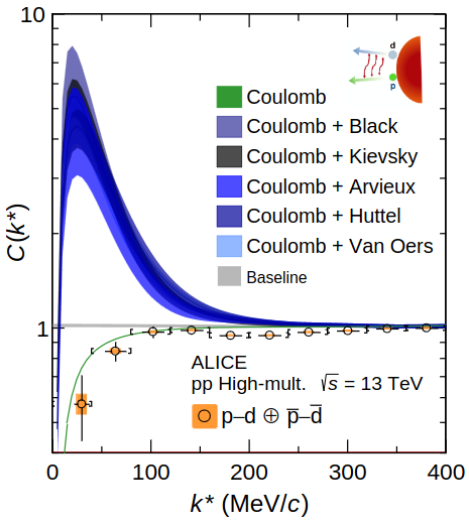

FIG. 6: Correlation functions calculated with the Lednický model for a source parameter $r_0 = (1.08 \pm 0.06)$ fm. Figure taken from Ref. [2] (ALICE collaboration).

In Fig. 6 we can observe the apparent discrepancy between the predictions of the Lednický model and the experimental data from ALICE [2]. The model described in this work fits better, as can be seen in Fig. 5.