Statistical nucleon correlation coefficients for the ^{3}H and ^{3}He nuclei

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The statistical nucleon correlation coefficients and a number of other properties for the ^{3}H and ^{3}He nuclei are calculated from highly accurate variational wave functions. Most of these properties were not considered previously. In particular, the two-body cusp conditions are obtained in general form for the Yukawa-type NN potential.

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In the present Brief Report we consider the bound states in the three-body nuclei ^{3}H and ^{3}He. Initially, our interest in these nuclei was related mainly to applications to fusion and annihilation processes in Coulomb three-body systems [1]. Indeed, in order to solve some problems related with applications to nuclear fusion [2] as well as with antiproton annihilation in few-body systems (e.g., in the $d^+t^+p^-$ system [1]) it is necessary, in particular, to calculate the basic properties of the three-particle ^{3}H and ^{3}He nuclei. However, most of the needed properties were not even discussed previously, and, therefore, cannot be found in the literature. Moreover, the results of such calculations strongly depend on the properties of the NN potential that is used.

We consider a number of geometrical and related properties for these nuclei, including the two-body cusp conditions and the so-called nucleon statistical correlation coefficients (SCC). These coefficients can be applied to study the statistical nucleon correlation in ^{3}H and ^{3}He. They show the difference between the particle pair density and the product of one-particle densities. For systems of completely independent particles, SCC must vanish or be equal to the numerical values which are known *a priori*. These coefficients had been introduced for the first time in atomic calculations [3]. Later they were applied successfully to the analysis of various Coulomb bound systems: atoms and ions [4], molecules [5], mesomolecules, and so-called exotic systems [1], [6]. Their values are of interest for understanding NN interactions as well as for the general theory of bound states in few-body systems.

The choice of the NN potential is central to a study of few-nucleon systems. As is well known there are two different approaches to reconstruct the potential of the nucleon-nucleon interaction. In the first method experimental two-nucleon data from elastic NN scattering are used (see, e.g., [7] and [8]). The so-called realistic NN potentials obtained have a very complicated structure and calculations with them are quite difficult to carry out. In addition to this, by applying these realistic NN potentials it is impossible to reproduce with good accuracy some of the characteristics of three-particle nuclei. Highly accurate variational calculations of the three-nucleon systems with realistic NN potentials can be found, e.g., in [9–11]. In other works [12–15] the Faddeev method was applied successfully to the same systems. It should be mentioned that probably the best variational results for the three-nucleon systems were obtained by an originally coupled-channel variational procedure proposed in [16]. Also, in that work three-nucleon forces were considered. Further discussion on the modern status of highly accurate calculations with realistic NN potentials can be found, e.g., in [9]. In the other approach (see, e.g., [17] and [18]) NN potentials of simple form are used which have been subsequently corrected in terms of the NN scattering and deuteron data. However, in this method the binding energies and the properties of the ^{3}H and ^{3}He nuclei cannot be found simultaneously with good accuracy. This means that neither of these approaches are able to describe those properties of the three-particle nuclei which are needed in some applications.

In the present study, we propose a different approach to this problem. In this method simple forms for the NN potential are also used. Initially they were taken from papers corresponding to the second approach mentioned above. Then some of the potential parameters were adjusted to describe "quite well" the basic nonscattering properties of the three-body nuclei, e.g., the energies, geometric, and related parameters. In other words the energy is considered only as one of the parameters which are determined in the calculations. The considered NN potential must be able to reproduce the nuclear properties with relatively good accuracy. Obviously this approach is more convenient in applications where the three-body nuclei are parts of many-particle systems. It should be emphasized that in contrast to the previous works we consider approximately three dozen independent properties for each of the ^{3}H and ^{3}He nuclei. Such a large number of nuclear properties for each nucleus is studied for different choices of the NN potential. In principle, by applying this approach to the different forms of the NN potential we can reconstruct better the unknown potential of the nucleon-nucleon interaction.

Throughout this paper we have used the following values for the physical constants $\frac{\hbar}{2m_p} = 20.749822$ MeV fm^2, $e^2 = 1.439965173$ MeV fm and $x = \frac{m_n}{m_p} = 939.565\,63/$

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938.272 31 = 1.001 378 406. The values of c, $\hbar$, a_0 as well as the proton m_p and neutron m_n masses were taken from CODATA 1986 (see, e.g., [19]). In the present paper all energies are expressed in MeV and distances in fm.

The ansatz for the wave function used in the present variational calculations of the $S(L=0)$ ground states is

$$\psi(r_{32}, r_{31}, r_{21}) = (1 + P_{21}) \sum_{i=1}^{N} C_i \exp(\alpha_i r_{32} - \beta_i r_{31} - \gamma_i r_{21}), \quad (1)$$

where 1 and 2 are identical particles, P_{21} is the permutation operator, and r_{ij}, $(ij) = (32), (31), (21)$, are three interparticle distances (relative coordinates). This exponential variational expansion was applied for the first time to nuclear three-body problems by Dalitz and Downs [22]. In our calculations the linear parameters C_i $(i = 1, 2, \ldots, N)$ are determined variationally. The nonlinear parameters $\alpha_i, \beta_i, \gamma_i$ are selected quasirandomly [20] from three positive intervals $[0, A], [0, B], [0, G]$. The values of the constants A, B, and G were chosen as 2.07, 2.17, and 1.95, respectively. Such a quasirandom choice of α_i, β_i, and γ_i requires computational times which are negligibly short in comparison with the alternative approach [21] of stepwise optimization. In the present calculations we have used the trial wave function, Eq. (1), with the total number of basis functions N up to 600.

The two following effective (i.e., spin averaged) potentials $V(r_{ij})$ were used to describe the nucleon-nucleon interaction:

$$V(r_{ij}) = A_+ \frac{\exp(-k_+ r_{ij})}{r_{ij}} + A_- \frac{\exp(-k_- r_{ij})}{r_{ij}} + \frac{q_i q_j}{r_{ij}}, \quad (2)$$

where q_i $(i = 1, 2, 3)$ are the charges of the nucleons and the $A_\pm = \frac{1}{2}(A^t_\pm + A^s_\pm)$ with $A^{t,s}_\pm$ the amplitudes of the interaction potential in the triplet and singlet states, respectively. Each of the NN potentials, Eq. (2), is a Yukawa-type potential, or, in other words, it has the so-called Malfliet-Tjon form [17]. The potential parameters were chosen to be $A^t_+ = 1438.68$ MeV fm, $A^s_+ = 1438.67$ MeV fm, $k_+ = 3.11$ fm^{-1}, $A^t_- = -626.86$ MeV fm, $A^s_- = -522.70$ MeV fm, $k_- = 1.55$ fm^{-1} for the first (I) case, and $A_+ = 0, A_- = -63.795\,567$ MeV fm, $k_- = 0.858138$ fm^{-1}, for the second (II) case. The last choice coincides with the NN potential used in [23]. Our numerical results for the first and second potential are given in Tables I and II, respectively. As expected our energies calculated with more extensive wave functions are lower than the previously calculated [23] energies (for 20 basis functions) with potential (II): ≈ -8.56 MeV (^{3}H) and ≈ -7.47 MeV (^{3}He).

The properties of the ^{3}H and ^{3}He nuclei for both potentials are listed in the tables. In these tables $\langle \delta(\mathbf{r}_{ij}) \rangle$ is the expectation value of the appropriate Dirac δ function. The expectation value of the two-body cusp ratio ν_{ij} between particles i and j is $\nu_{ij} = \langle \delta(\mathbf{r}_{ij}) \times (\partial/\partial r_{ij}) \rangle / \langle \delta(\mathbf{r}_{ij}) \rangle$. In contrast with Coulomb systems (see, e.g., [24], [25]) the "exact" values of the ν_{ij} in the real nuclear systems ^{3}H and ^{3}He are unknown because the "exact" potential is unknown. The cusp value with the exact wave function for the Yukawa-type potentials in the form of Eq. (2) must equal $\mu_{ij}(A_+ + A_- + e^2 q_i q_j)(m_p/\hbar)$ fm^{-1} where $\mu_{ij} = \frac{m_i m_j}{m_i + m_j} \approx 0.5$, $q_p = +1, q_n = 0$. The values m_i and m_j coincide with m_n and (or) m_p. In the units used ($m_p = 1$, $m_n = x$) the last equation takes the form $\nu_{ij} = \mu_{ij}(0.024\,096\,592\,25(A_+ + A_-) + 0.034\,698\,253\,6 q_i q_j)$ fm^{-1}. Thus, $\nu_{ij} = 0.012\,064\,903\,57(A_+ + A_-)$ fm^{-1} for the nn cusp, $\nu_{ij} = 0.012\,056\,594\,13(A_+ + A_-)$ fm^{-1} for the np cusp, and $\nu_{ij} = [0.012\,048\,296\,13(A_+ + A_-) + 0.017\,349\,126\,82]$ fm^{-1} for the pp cusp.

TABLE I. The expectation values of the various properties for the ^{3}H and ^{3}He nuclei with the first (I) choice of the NN-potential parameters.

	nnp	*ppn*		*nnp*	*ppn*
	123	123		123	123
$\langle r_{21} \rangle$	2.55753	2.60598	$\langle r_{31} \rangle$	2.55835	2.58346
$\langle r^2_{21} \rangle$	8.31568	8.66580	$\langle r^2_{31} \rangle$	8.32119	8.51304
$\langle r^3_{21} \rangle$	33.4671	35.7922	$\langle r^3_{31} \rangle$	33.5011	34.8336
$\langle r^4_{21} \rangle$	162.769	179.194	$\langle r^4_{31} \rangle$	163.020	172.7735
$\langle r^{-1}_{21} \rangle$	0.512333	0.504685	$\langle r^{-1}_{31} \rangle$	0.512198	0.508751
$\langle (r_{31} r_{21})^{-1} \rangle$	0.280433	0.275035	$\langle (r_{31} r_{32})^{-1} \rangle$	0.280386	0.276512
$\langle (\mathbf{r}_{31} \cdot \mathbf{r}_{32}) \rangle$	4.16335	4.18014	$\langle (\mathbf{r}_{31} \cdot \mathbf{r}_{21}) \rangle$	4.15784	4.33290
$\langle \nabla_1 \cdot \nabla_2 \rangle$	2.74097	2.67929	$\langle \nabla_1 \cdot \nabla_3 \rangle$	2.74097	2.68440
$\langle \frac{1}{2} \nabla^2_1 \rangle$	10.3613	10.3675	$\langle \frac{1}{2} \nabla^2_3 \rangle$	10.3676	10.3613
$\langle \delta_{21} \rangle \times 10^{-3}$	0.18914	0.18002	$\langle \delta_{31} \rangle \times 10^{-3}$	0.18739	0.18457
$\langle \delta_{321} \rangle \times 10^{-6}$	0.29020	0.24488			
ν_{21}	10.3367	10.3358	ν_{31}	10.5366	10.5247
ν_{21}[a]	10.4228	10.4258	ν_{31}[a]	10.4156	10.4156
$\langle T \rangle$	31.0678	30.4349	$\langle V \rangle$	−39.5438	−38.1646
E	−8.475949	−7.729693	χ	0.21434	0.20254

[a]The exact value for potential parameters (I).

TABLE II. The expectation values of the various properties for the ^{3}H and ^{3}He nuclei with the second (II) choice of the NN-potential parameters.

	nnp	*ppn*		*nnp*	*ppn*
	123	123		123	123
$\langle r_{21}\rangle$	2.03521	2.11079	$\langle r_{31}\rangle$	2.03601	2.08645
$\langle r_{21}^2\rangle$	5.70375	6.16097	$\langle r_{31}^2\rangle$	5.70814	6.02230
$\langle r_{21}^3\rangle$	20.65112	23.32282	$\langle r_{31}^3\rangle$	20.67468	22.55063
$\langle r_{21}^4\rangle$	92.6089	109.7319	$\langle r_{31}^4\rangle$	92.7476	104.9706
$\langle r_{21}^{-1}\rangle$	0.758128	0.734036	$\langle r_{31}^{-1}\rangle$	0.757815	0.743219
$\langle (r_{31}r_{21})^{-1}\rangle$	0.680113	0.649067	$\langle (r_{31}r_{32})^{-1}\rangle$	0.679948	0.653579
$\langle (\mathbf{r}_{31}\cdot\mathbf{r}_{32})\rangle$	2.85627	2.94182	$\langle (\mathbf{r}_{31}\cdot\mathbf{r}_{21})\rangle$	2.85187	3.08049
$\langle \nabla_1\cdot\nabla_2\rangle$	4.99904	4.75748	$\langle \nabla_1\cdot\nabla_3\rangle$	4.99897	4.78290
$\langle \frac{1}{2}\nabla_1^2\rangle$	17.0551	16.1887	$\langle \frac{1}{2}\nabla_3^2\rangle$	17.0429	16.5187
$\langle \delta_{21}\rangle$	0.14509	0.13305	$\langle \delta_{31}\rangle$	0.14489	0.13903
$\langle \delta_{321}\rangle$	0.10463	0.09495			
ν_{21}	−0.76959	−0.75118	ν_{31}	−0.76916	−0.76919
ν_{21}[a]	−0.76969	−0.75128	ν_{31}[a]	−0.76915	−0.76915
$\langle T\rangle$	51.10614	48.87329	$\langle V\rangle$	−59.72596	−56.39605
E	−8.619825	−7.522758	χ	0.14432	0.13339

[a]The exact value for potential parameters (II).

The cusp ratios test the accuracy of wave functions near points of coalescence of two nucleons and the real "exact" values must be deduced from the nucleon structure as reflected in the potential. For the present potentials our solutions are quite good there, since the calculated cusp values lie very close to the cusp ratios predicted above.

The dimensionless parameter $\chi = 1 + \langle T\rangle/\langle V\rangle = E/\langle V\rangle$ [where T (V) is the kinetic (potential) energy operator] is the ratio of the bound state energy E to the effective depth $\langle V\rangle$ of the potential well. For these systems with both E and $\langle V\rangle$ negative we expect $0 \le \chi \le 1$.

Now, consider the statistical nucleon-nucleon correlation in the ^{3}H and ^{3}He nuclei as measured by the SCC. In Table III the statistical angular correlation coefficients are $\tau_{ij} = \langle \hat{\mathbf{r}}_{ik}\cdot\hat{\mathbf{r}}_{jk}\rangle$ where $\hat{\mathbf{r}} = \mathbf{r}/r$ and $(ij),(ik),(jk) =$ (21), (31), and (32). It should be noted that the value of an arbitrary SCC must be bounded between +1 and −1. If $\tau_{ij} = +1$ there is perfect positive correlation where the position vectors of nucleons i and j (i.e., $\mathbf{r}_{ik}$ and $\mathbf{r}_{jk}$) are expected to coincide and if $\tau_{ij} = -1$ there is perfect negative correlation where particles i and j are expected to be at diametrical positions with respect to the third particle k. Note that in the ^{3}H and ^{3}He nuclei $\tau_{32} = \tau_{31} \approx \tau_{21}$ (in contrast with atomic and exotic systems [6] where they differ significantly).

In addition to τ_{ij}, we have calculated two other statistical angular correlation coefficients, $\tau_{\mathbf{r}_{ij}} = 2\langle \mathbf{r}_{ik}\cdot\mathbf{r}_{jk}\rangle/\big(\langle \mathbf{r}_{ik}^2\rangle + \langle \mathbf{r}_{jk}^2\rangle\big)$ and $\tau_{\mathbf{p}_{ij}} = 2\langle \nabla_i\cdot\nabla_j\rangle/\big(\langle \nabla_i^2\rangle + \langle \nabla_j^2\rangle\big)$. It should be noted that τ_{ij} ($\tau_{\mathbf{r}_{ij}}$) assesses angular correlation primarily for small (intermediate) separations of the third nucleon from i and j, while $\tau_{\mathbf{p}_{ij}}$ assesses angular correlation for intermediate momenta $\mathbf{p}_{ij}$. Since in both nuclei $\langle r_{31}^2\rangle = \langle r_{32}^2\rangle \approx \langle r_{21}^2\rangle$, we have

$$\tau_{\mathbf{r}_{ij}} = \frac{\langle \mathbf{r}_{ik}^2\rangle + \langle \mathbf{r}_{jk}^2\rangle - \langle \mathbf{r}_{ij}^2\rangle}{\langle \mathbf{r}_{ik}^2\rangle + \langle \mathbf{r}_{jk}^2\rangle} \approx \frac{\langle \mathbf{r}_{ik}^2\rangle}{2\langle \mathbf{r}_{ik}^2\rangle} \approx 0.5. \qquad (3)$$

The values of $\tau_{\mathbf{r}_{np}}$ and $\tau_{\mathbf{r}_{pp}}$ must be greater than 0.5 and less than 0.5, respectively, for the ^{3}He nucleus, since the inequality $\langle r_{pp}^2\rangle > \langle r_{np}^2\rangle$ is obeyed due to the Coulomb repulsion between the pair of protons.

The dimensionless Pearson correlation coefficients Δ_{ij} in Table III are $\Delta_{ij} = \sqrt{\langle r_{ij}^2\rangle - \langle r_{ij}\rangle^2}/\langle r_{ij}\rangle$. These coefficients can be used as a measure of the uncertainty in the expected geometrical structure.

Most of the properties presented in the tables are quite sensitive to the shape of the NN potential used. In particular, the expected triangular geometries of ^{3}H and ^{3}He nuclei are about the same for the potential (I) with the same percent uncertainty ($\approx$ 50%). For potential (II)

TABLE III. Comparision of the statistical correlation and Pearson coefficients for the ^{3}H and ^{3}He nuclei and for the Ps^- ion.

	nnp	*ppn*	$e^-e^-e^+$
	123	123	1 2 3
τ_{21}	0.433885[a]	0.426783[a]	0.019770
	0.427678[b]	0.419391[b]	
τ_{31}	0.433498[a]	0.436799[a]	0.591982
	0.427232[b]	0.431227[b]	
$\tau_{\mathbf{r}_{21}}$	0.500331[a]	0.491028[a]	0.037787
	0.500385[b]	0.488487[b]	
$\tau_{\mathbf{r}_{31}}$	0.499834[a]	0.504446[a]	0.658052
	0.499807[b]	0.505691[b]	
$\tau_{\mathbf{p}_{21}}$	0.132229[a]	0.129501[a]	0.012976
	0.146556[b]	0.146939[b]	
$\tau_{\mathbf{p}_{31}}$	0.132270[a]	0.129216[a]	0.016239
	0.146605[b]	0.146233[b]	
Δ_{21}	0.520888[a]	0.525401[a]	0.524455
	0.614022[b]	0.618710[b]	
Δ_{31}	0.520914[a]	0.524883[a]	0.778895
	0.614008[b]	0.619191[b]	

[a]These data correspond to the first (I) choice of the NN-potential parameters.
[b]These data correspond to the second (II) choice of the NN-potential parameters.

the expected geometries of ^{3}H and ^{3}He are similar, but considerably smaller than for potential (I). As expected for both potentials, ^{3}H is slightly smaller in size than ^{3}He. The uncertainties for the potential (II) are larger ($\approx 60\%$) than for potential (I). In contrast with these geometrical properties the nucleon SCC (Table III) are nearly the same for both potentials. Therefore, it seems reasonable to assume that these SCC will not change significantly for a heavier nucleus. In other words, based on these numerical values we can predict some other geometric and related properties of such a nucleus. Also, it follows from Table III that an arbitrary neutron-neutron SCC is approximately equal to the respective value of the neutron-proton SCC as well as proton-proton SCC.

Since the nucleon SCC are dimensionless quantities, they can be compared directly with the SCC in the atomic and exotic Coulomb three-body systems. In the case of the Ps^- (or $e^-e^-e^+$) ion such a comparison is interesting for the general theory of bound states in three-body systems. Indeed, in the Ps^- ion all masses are equal to each other and it has only one bound state. Therefore, the difference in the properties can be explained only by the difference in the pair potentials. The basic properties for the Ps^- ion are given in [6]. The numerical comparison of the nucleon SCC for both nuclei with the SCC in the Ps^- ion is given in Table III. SCC for the Ps^- ion were calculated for the trial wave function Eq. (1) with $N = 850$ [6]. Note that in contrast to the considered three-nucleon systems, the electron-electron SCC in the Ps^- ion differs significantly from the electron-positron SCC. This means that Ps^- has a definite cluster structure while the ^{3}H and ^{3}He nuclei do not. Actually the Ps^- ion consists essentially of the two-body neutral cluster Ps (e^-e^+) and the other electron (e^-) which moves far away from it. In both of these nuclei the structure cannot be represented in terms of a two-body cluster model.

Thus, in the present study we have considered the properties of the three-body ^{3}H and ^{3}He nuclei in their bound ground states with the use of the highly accurate exponential wave function, Eq. (1), in the relative coordinates r_{32}, r_{31}, and r_{21}. The two-body cusp condition for an arbitrary Yukawa-type potential has been formulated. It can be applied to test independently the accuracy of trial wave functions used in variational calculations. The statistical nucleon correlation coefficients (SCC) have been calculated and discussed for both these nuclei. The nucleon-nucleon SCC have been compared with the appropriate SCC values in the Coulomb three-body Ps^- ion. The results of our present calculations suggest that, on the basis of a few dozen properties, it is possible, in principle, to make a more correct choice between the different types of NN potentials.

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