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Phys. Rev. C **108**, L021301 — Published 2 August 2023

DOI: 10.1103/PhysRevC.108.L021301

LA-UR-22-32748

Nuclear three-body short-range correlations in coordinate space

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(Dated: July 13, 2023)

We study the effects of three-nucleon short-range correlations on nuclear coordinate-space densities. For this purpose, novel three-body densities are calculated for ground state nuclei using the auxiliary-field diffusion Monte Carlo method. The results are analyzed in terms of the Generalized Contact Formalism, extended to include three-body correlations, revealing the universal behavior of nucleon triplets at short distances. We identify the quantum numbers of such correlated triplets and extract scaling factors of triplet abundances that can be compared to upcoming inclusive electron scattering data. We also show that the dynamics of these triplets is sensitive to three-body forces, and, therefore, the short-range part of three-body force models could be tested against appropriate exclusive electron scattering data.

Short-range correlations (SRCs) are an integral part of the description of strongly interacting many-body quantum systems. Strong SRCs lead to significant deviations from non-interacting models, *e.g.*, by inducing high-momentum components in the wave function, and, therefore, pose a challenge in the description of such systems.

The largest effects of SRCs are due to pairs of particles that are found close together inside the many-body system. Such pairs have been studied thoroughly in the last decades in different systems. The so-called *contact* theory was developed and used to reveal universal relations between quantities affected by SRCs assuming zero-range interaction [1–5], which were verified experimentally in ultracold atomic systems [6–10]. SRCs were also studied for the case of Helium atoms [11]. In nuclear systems [12–14], SRC pairs have been studied mainly via large momentum transfer quasi-elastic electron- and proton-scattering experiments [15–35], and ab-initio many-body calculations [36–45], establishing the universal features of such pairs and the dominance of neutron-proton (np) pairs.

The properties of SRC pairs in different systems are similar. Generally, two particles at short distances behave as an isolated system, unaffected by the remaining particles in the system. In momentum space, they are mostly in back-to-back configuration and are the leading source of high-momentum particles in the system. Accounting for their effects is important for an accurate description of different observables, like electron and neutrino scattering cross sections [46–50] and neutrinoless double beta decay matrix elements [51–53] in nuclear systems, or the structure factor of liquid ^{4}He [11].

Unlike pairs, the features and importance of SRC triplets are much less understood. Some properties of triplets have been studied for the case of zero-range interactions [54, 55] and Helium atoms [11]. For nuclei, there are currently significant efforts to study such correlated triplets experimentally [56–58], but there has been no clear identification of three-nucleon SRCs. Similarly, nuclear many-body ab-initio calculations that allow direct access to triplet properties have not been performed so far. Theoretical studies of three-nucleon SRCs are important for guiding the experimental efforts and data analysis and for revealing the properties and impact of such triplets. In this work we focus on nuclear systems, but like the case of two-body SRCs, the conclusion and methods of this work should be relevant also for other systems.

Following the development of the contact theory for zero-range interactions [1–5], the Generalized Contact Formalism (GCF) was introduced to study nuclear SRCs [59–63]. The GCF is based on the realization that when two nucleons are close to each other in a nucleus with A nucleons, the many-body wave function Ψ factorizes to a two-body part, describing the correlated pair, and a function describing the rest of the nucleons in the system [60]

$$\Psi \xrightarrow[r_{ij}\to 0]{} \sum_{\alpha} \varphi^{\alpha}(\boldsymbol{r}_{ij}) A^{\alpha}(\boldsymbol{R}_{ij}, \{\boldsymbol{r}_k\}_{k\neq i,j}). \tag{1}$$

Here, $\boldsymbol{r}_k$ denotes the single-nucleon coordinate, $\boldsymbol{r}_{ij} \equiv \boldsymbol{r}_j - \boldsymbol{r}_i$ and $\boldsymbol{R}_{ij} \equiv (\boldsymbol{r}_i + \boldsymbol{r}_j)/2$ are the relative and center-of-mass (CM) coordinates, and α denotes the quantum numbers of the pair. $\varphi^{\alpha}(\boldsymbol{r}_{ij})$ describes the dynamics of the correlated pair and is defined as the solution of the zero-energy two-body Schrödinger equation. As such it is universal, *i.e.* nucleus independent, but depends on the nucleon-nucleon interaction model. The function A^{α} describes the rest of the particles in the system when particles i and j are close together. This factorization was verified using ab-initio calculations [60, 64–66], and is supported by renormalization-group arguments [67–69] and the Coupled-Cluster expansion [70].

The factorization of Ψ is useful for describing the impact of two-nucleon SRCs on different observables. If we consider a short-range two-body operator $\hat{O}$, its expectation value $\langle \hat{O} \rangle$ would be of the form

$$\langle \Psi | \hat{O} | \Psi \rangle = \sum_{\alpha,\beta} \langle \varphi^{\alpha} | \hat{O} | \varphi^{\beta} \rangle C_2^{\alpha\beta}, \tag{2}$$

where $C_2^{\alpha\beta} \equiv A(A-1)/2 \times \langle A^{\alpha} | A^{\beta} \rangle$ are the nuclear contacts; they measure the probability of two particles

to be close together. Notice that $C_2^{\alpha\beta}$ is independent of $\hat{O}$. Therefore, different observables are all described with the same contact parameters. The matrix elements $\langle\varphi^\alpha|\hat{O}|\varphi^\beta\rangle$ provide the contribution of the pair to this observable. This matrix element is nucleus independent and involves only the two-body problem. One simple example is the two-body density $\rho_2(r)$, obtained by $\hat{O}=\delta(r_{ij}-r)$. Based on this approach, a comprehensive and consistent description of different quantities sensitive to two-body SRCs was obtained [25, 33–35, 48, 53, 59–61, 64, 65, 71–73].

We want to extend this description to three-body correlations in nuclear systems. The above two-body factorization is valid when none of the remaining $A-2$ nucleons is close to the correlated pair. If one nucleon is close enough to such a pair, *i.e.* when three nucleons are close to each other, we expect the many-body nuclear wave function to factorize in the following way

$$\Psi \xrightarrow[x_{ij},x_{ijl}\to 0]{} \sum_\beta \varphi_{ijl}^\beta(\boldsymbol{x}_{ij},\boldsymbol{x}_{ijl})B_{ijl}^\beta(\boldsymbol{R}_{ijl},\{\boldsymbol{r}_m\}_{m\neq i,j,l}). \tag{3}$$

We used here the Jacobi coordinates $\boldsymbol{x}_{ij}\equiv\boldsymbol{r}_j-\boldsymbol{r}_i$ and $\boldsymbol{x}_{ijl}\equiv\boldsymbol{r}_l-(\boldsymbol{r}_i+\boldsymbol{r}_j)/2$ and the triplet CM coordinate $\boldsymbol{R}_{ijl}\equiv(\boldsymbol{r}_i+\boldsymbol{r}_j+\boldsymbol{r}_l)/3$. φ_{ijl}^β describes the dynamics of the SRC triplet and is defined as a zero-energy solution of the three-body Schrödinger equation with quantum numbers given by β (with the same nuclear-interaction model used to define Ψ). The connection of three-nucleon SRCs to the zero-energy three-body eigenstates is discussed also in Ref. [70]. The function B_{ijl}^β describes the rest of the particles in the system when particles i,j and l are close together.

For realistic nuclear interactions, each channel β is defined by the quantum numbers $\beta=(\pi_\beta,j_\beta,m_\beta,t_\beta,t_{z,\beta})$, where π_β is the parity, j_β and m_β are the total angular momentum and its projection, and t_β and $t_{z,\beta}$ are the total isospin of the triplet and its projection (isospin is equivalent to spin for the description of protons and neutrons as identical particles with internal isospin degree of freedom). At short distances, we expect to see a dominant contribution of zero angular-momentum ($\ell=0$) states. Due to Pauli blocking, proton-proton-proton (ppp) and neutron-neutron-neutron (nnn) ($t=3/2$) triplets are expected to be suppressed at short distances compared to proton-proton-neutron (ppn) and proton-neutron-neutron (pnn) ($t=1/2$) triplets. spin-3/2 triplets are similarly suppressed. Therefore, we expect $\pi=+,j=1/2,t=1/2$ (and $m=\pm1/2$ and $t_z=\pm1/2$) to be the dominant channel for SRC triplets. This correspond to the quantum numbers of ^{3}He and ^{3}H ground states. Notice that while np dominance of two-body SRCs is caused by the tensor force [36, 37], here it is the Pauli principle that leads to $t=1/2$ dominance for three-body SRCs. See more details regarding the structure of φ_{ijl}^β and the dominant channels in the supplemental materials.

Similar to the two-body case, and based on Eq. (3), we can now define the three-nucleon contact matrix

$$C_3^{\beta\gamma}=\frac{A(A-1)(A-2)}{6}\langle B_{123}^\beta|B_{123}^\gamma\rangle. \tag{4}$$

The combinatorical factor is suitable assuming Ψ is fully anti-symmetric. Three-body contacts were similarly defined for the zero-range limit [54, 55] and for Helium atoms [11]. These three-body contacts describe the probability of finding three nucleons in close proximity inside a nucleus. See more details regarding the properties of the three-nucleon contact matrix in the supplemental materials.

To study the implications of such SRC triplets, we would like to derive relations similar to those derived for the case of two-body SRCs, based on Eq. (2). We consider in this work three-body densities in coordinate space. Specifically, we consider the three-body density describing the probability of finding three nucleons inside a nucleus in a triangle with sides of length r_{12}, r_{13} and r_{23}

$$\rho_3(r_{12},r_{13},r_{23})=\binom{A}{3}\left\langle\prod_{i<j=1}^{3}\delta(|\boldsymbol{r}_i-\boldsymbol{r}_j|-r_{ij})\right\rangle. \tag{5}$$

In the limit of $r_{12},r_{13},r_{23}\to 0$, we can use Eqs. (3) and (4) to obtain

$$\rho_3\to C_3^{t=1/2}\left\langle\varphi^{t=1/2}\left|\prod_{i<j=1}^{3}\delta(|\boldsymbol{r}_i-\boldsymbol{r}_j|-r_{ij})\right|\varphi^{t=1/2}\right\rangle. \tag{6}$$

We have considered here the contribution of the leading isospin-half channel, with the relevant contact denoted as $C_3^{t=1/2}$ and universal function as $\varphi^{t=1/2}$. Based on this result, we expect to find a universal behavior of ρ_3 at short distances for all nuclei, *i.e.* the same r-dependence with only a global scaling factor that depends on the nucleus. We can also consider isospin-projected densities ρ_3^t, by inserting the appropriate three-body projection operator in Eq. (5). For these quantities, we expect to see a dominance of $t=1/2$ over $t=3/2$ as discussed above.

In order to verify these GCF predictions regarding three-nucleons SRCs, we now turn to ab-initio calculations of $\rho_3(r_{12},r_{13},r_{23})$ for the ground-state nuclei ^{3}He, ^{4}He, ^{6}Li and ^{16}O. We used the auxiliary-field diffusion Monte Carlo (AFDMC) method [74, 75] combined with the N2LO local chiral interaction with the E1 parametrization of the three-body force [75–78]. We focus here on the $R_0=1.0$ fm cutoff but show also some results for $R_0=1.2$ fm.

We first start with investigating ρ_3^t in order to compare the $t=1/2$ and $t=3/2$ densities. The three-body

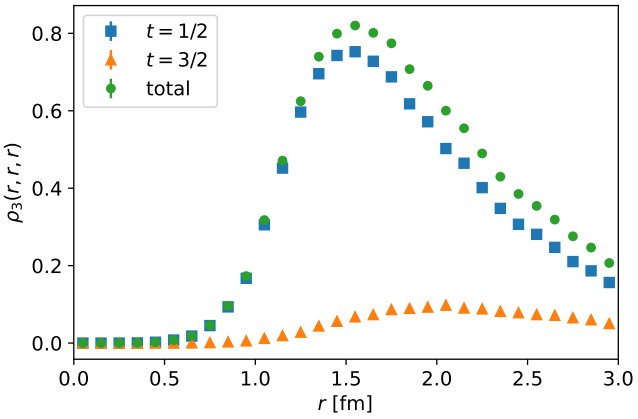


FIG. 1. ^{6}Li three-body density for equilateral triangles as a function of the triangle side using the AFDMC method and the N2LO(1.0) interaction. Projections to $t = 1/2$ and $t = 3/2$ triplets are shown together with the total density.

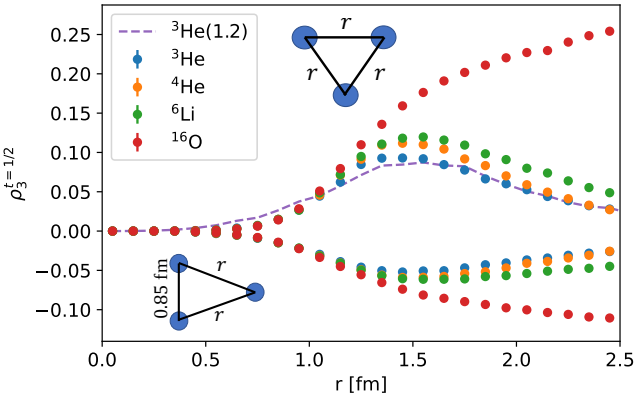


FIG. 2. AFDMC $\rho_3^{t=1/2}$ densities for ^{3}He, ^{4}He, ^{6}Li and ^{16}O for both equilateral triangle and isosceles triangle using the N2LO(1.0) interaction (circles). For the latter, the base is fixed at length of 0.85 fm and the densities are multiplied by minus one (see text for details). The ^{4}He, ^{6}Li and ^{16}O densities are each multiplied by a scaling factor (the same factor for both geometries). ^{3}He equilateral-triangle density is shown also for the N2LO(1.2) interaction (dashed line).

density for ^{6}Li is shown in Fig. 1 for equilateral triangles, *i.e.* $\rho_3(r,r,r)$ as a function of r. We can clearly see that at short distances the $t = 1/2$ component is indeed dominant. As r increases the contribution of $t = 3/2$ triplets grows, and a similar behavior is seen for other geometries, *e.g.*, isosceles triangles, and also for ^{16}O (see supplemental materials). .

Based on Fig. 1, we can also see that the total number of $t = 3/2$ triplets in ^{6}Li is much smaller than $t = 1/2$ triplets. In addition, ^{3}He and ^{4}He include only $t = 1/2$ triplets. This could have implications for the fitting of three-nucleon forces. In fact, in most of the cases, three-nucleon interactions are fitted to such light systems where the $t = 3/2$ component is either zero or very small (see for example Refs. [78–80]). In order to account for $t = 3/2$ physics, fitting to larger nuclei like ^{16}O could be beneficial as the $t = 3/2$ component is larger (see supplemental materials). This can be relevant for the description of the Equation of State inside neutron stars and properties of neutron-rich nuclei, for which *nnn* physics is important.

We can now focus on the $t = 1/2$ component and compare the behavior of different nuclei. We present in Fig. 2 the density $\rho_3^{t=1/2}$ for all available nuclei for both equilateral and isosceles triangle geometries using the N2LO(1.0) interaction. For the isosceles triangle, we fix the base to be of length $a = 0.85$ fm. The ^{4}He, ^{6}Li and ^{16}O calculations are rescaled so that their shape at short distances can be compared to ^{3}He. Only for plotting purposes, the densities of the isosceles triangle are multiplied by minus one to separate them from the equilateral-triangle results. We can see that, for each of the geometries, the r-dependence of $\rho_3^{t=1/2}$ is the same at short distances ($r \lesssim 1.1$ fm) for all nuclei, as all densities coincide with the ^{3}He density. This shows the universal behavior of SRC triplets as predicted by the GCF. Indeed, a single $t = 1/2$ channel is dominant here (otherwise the densities would not coincide) due to the dominance of $\ell = 0$ at short distances. It should be emphasized that the same scaling factor is applied to both the equilateral and isosceles cases for each nucleus, in agreement with Eq. (6). The same behavior is seen for other configurations involving three particles close together. This result is an important validation of the asymptotic three-body factorization of the many-body wave function, Eq. (3). We also include in Fig. 2 the ^{3}He equilateral-triangle density using the N2LO(1.2) interaction. We can see that the short-distance behavior in this case is different. This shows that the three-body wave functions of the GCF φ_{ijl}^{β} indeed depend on the model of the interaction. We note that universal behavior is also seen in the $t = 3/2$ density, indicating that asymptotic factorization holds also for $t = 3/2$ triplets with a single dominant channel (see supplemental materials).

The scaling factor used in Fig. 2 is equal to the contact value of Eq. (6) (relative to ^{3}He). As mentioned above, such contact values are proportional to the probability of finding correlated triplets in a given nucleus. There are ongoing experimental efforts to extract such probabilities using large momentum transfer quasi-elastic inclusive electron-scattering experiments [56]. For this purpose, a cross section ratio can be defined as [58]

$$a_3(A,Z) = \frac{3}{A}\frac{\sigma_{eA}}{(\sigma_{e^3\mathrm{He}} + \sigma_{e^3\mathrm{H}})/2}, \qquad (7)$$

where σ_{eA} is the inclusive electron-scattering cross section off nucleus A (with A nucleons, Z protons) at kinematics dominated by three-body SRCs. Interpreting a_3

contact ratio	$A=4$	$A=6$	$A=16$
$t=1/2$	3.8 ± 0.3	3.1 ± 0.3	4.2 ± 0.5
$t=3/2$	-	-	5.4 ± 0.8

TABLE I. Per nucleon three-body contact ratio for $t=1/2$ (with respect to ^{3}He) and for $t=3/2$ (with respect to ^{6}Li), *i.e.* $\frac{3}{A}\frac{C_3^{t=1/2}(A)}{C_3^{t=1/2}(^3\mathrm{He})}$, and $\frac{6}{A}\frac{C_3^{t=3/2}(A)}{C_3^{t=3/2}(^6\mathrm{Li})}$, respectively.

as the ratio of three-nucleon SRC abundances, we obtain

$$a_3(A,Z)=\frac{3}{A}\frac{C_3^{t=1/2}(A)}{C_3^{t=1/2}(^3\mathrm{He})}, \tag{8}$$

for a symmetric nucleus A. We consider here only the leading contribution of $t=1/2$ triplets. It should be noted that, similar to the case of two-body SRCs [72], different effects can influence this interpretation of a_3, such as the CM motion of triplets, excitation energy of the $A-3$ system and contribution of $t=3/2$ triplets. In addition, for the case of non-symmetric nuclei or if using only ^{3}He cross section in the denominator, a more careful analysis of the reaction is needed because of different contributions of *ppn* and *nnp* triplets in the numerator and denominator.

Contact ratios extracted from the AFDMC calculations are presented in Table I. Their values were fitted to the equilateral three-body density based on Eq. (6) and its equivalent for the $t=3/2$ component. Since we are looking on contact ratios, there is no need to calculate the functions φ_{ijl}^{β}. Uncertainties were estimated by varying the lower and upper limits of the fitting range between $0.1-0.4$ fm and $1-1.2$ fm, respectively. The $t=1/2$ contact ratio provides a prediction for the value of a_3 for ^{4}He, ^{6}Li and ^{16}O. We can see that the per-nucleon $t=1/2$ ratios for ^{4}He and ^{16}O are similar, consistent with a ^{4}He-cluster structure of ^{16}O. It is also interesting to note that the per-nucleon $t=1/2$ ratio for ^{6}Li is smaller than that of ^{4}He. Results for additional nuclei are needed in order study the A-dependence of a_3.

In a recent work [58, 81, 82], Sargsian *et. al.* suggested a connection between two-body and three-body abundances, leading to a value of $a_3(^4\mathrm{He})\approx 3.15$. This is smaller than the value we obtained here (Table I). We emphasize that in the GCF approach three-nucleon abundances are generally independent of two-nucleon abundances. Large momentum transfer quasi-elastic inclusive electron-scattering experiments sensitive to three-nucleon SRCs might be able to clear this issue.

One of the interesting questions about three-body SRCs is their connection to the three-body force. We investigate here this question by comparing calculations with and without a three-body force. The ratio of such calculations for equilateral triangle is shown in Fig. 3. We can see that there is no plateau at short distances (blue squares), showing that the universal function $\varphi^{t=1/2}$ is affected by the three-body force. In other words, the three-body force impacts the dynamics of SRC triplets. Ratios in which three body force is included (or not included) in both numerator and denominator are shown for comparison. In these cases a plateau is seen. Similar results are obtained for other geometries (see supplemental materials). We can, therefore, conclude that the three-body force plays an active role in the formation of three-nucleon SRCs. This also means that the theoretical description of exclusive electron-scattering reactions, in which momentum dependence of SRC triplets can be measured, will depend on the model of the three-body force at short distances.

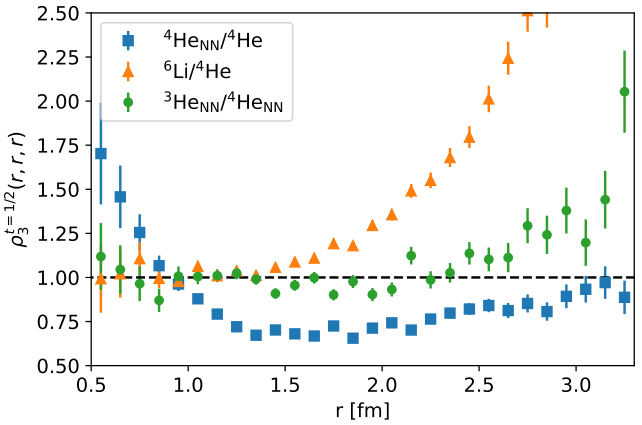


FIG. 3. Ratios of AFDMC calculations of $\rho_3^{t=1/2}$ for equilateral triangle using the N2LO(1.0) interaction. Calculations in which the three-body force is not included are denoted by 'NN'. The ratios were rescaled to be approximately 1 at short distances (using the contact values of Table I for the ^{6}Li/^{4}He ratio). ^{4}He was chosen as the reference nucleus (*i.e.* in the denominator) due to the small associated uncertainties.

To summarize, we have studied here the properties of three-nucleon SRCs in coordinate space. The GCF was extended to include correlated triplets, described as an isolated and universal subsystem within the many-body nucleus. The leading $t=1/2$ channel was identified and three-nucleon contacts were defined. Using novel AFDMC ab-initio calculations of three-body densities, the $t=1/2$ dominance and universality of such triplets at short distances was established numerically. Specifically, we found that three nucleons at short distances behave like the bound ^{3}He wave function. We have also extracted the values of the leading $t=1/2$ and $t=3/2$ contact ratios, describing the scaling of SRC triplet abundances. The connection to inclusive electron-scattering cross sections was discussed.

Finally, we have also shown that the three-body force is affecting the dynamics of SRC triplets. This provides further motivation for exclusive electron-scattering experiments in kinematics sensitive to three-nucleon SRCs.

Such experimental data will be sensitive to the short-range part of the three-nucleon force, important, *e.g.*, for neutron-star properties [83].

This work opens the path for additional studies of SRC triplets, including their impact on two-body densities, momentum distributions, spectral functions, electron and neutrino scattering off nuclei and neutrinoless double beta decay matrix elements. This is also an important step towards a systematic short-range expansion of the nuclear wave function. The methods used in this work could be relevant also for studies of SRCs in other systems like ultra-cold atomic gases.

We would like to thank J. Carlson, J. Martin, S. Novario, I. Tews, N. Barnea, B. Bazak, S. Beck, and E. Piasetzky for helpful discussions. The work of R.W. was supported by the Laboratory Directed Research and Development program of Los Alamos National Laboratory under project number 20210763PRD1. The work of S. G. was supported by U.S. Department of Energy, Office of Science, Office of Nuclear Physics, under Contract No. DE-AC52-06NA25396, by the DOE NUCLEI SciDAC Program, and by the DOE Early Career Research Program. Computer time was provided by the Los Alamos National Laboratory Institutional Computing Program, which is supported by the U.S. Department of Energy National Nuclear Security Administration under Contract No. 89233218CNA000001.

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