ON THE TRIPLET CORRELATION EFFECTS IN THE TRIMER ^{4}He

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An explicit expression for the triplet Feenberg function in r-space is obtained. Making use of this result and employing the variational ansatz the ground state energy of boson ^{4}He trimer, interacting via Lennard-Jones (12—6) pair potential, is evaluated. The ^{4}He trimer is considered because it includes triplet Feenberg correlations in the simplest form. It is shown that the binding energy is not improved after the inclusion of the triplet Feenberg function. In addition, the applicability of the approximation of averaging over equal interatomic distances is also discussed.

1. Introduction

The investigations of many-body correlations in many-body systems ($N \to \infty$, $\Omega \to \infty$, where N is the number of particles and Ω the volume of the system), which were omitted in Jastrow's two-body functions, started about ten years ago. Many-body correlations are described in Feenberg's function[1-5]

$$\psi \left(1, 2, \ldots N \right) = \exp \left\{ - \frac{1}{2} \, \bar{u}_N \left(1, 2, \ldots N \right) \right\}, \qquad (1)$$

where

$$\bar{u}_N \left(1, 2, \ldots N \right) = \sum_{i<j} u_2 \left(\vec{r}_i, \vec{r}_j \right) + \sum_{i<j<k} u_3 \left(\vec{r}_i, \vec{r}_j, \vec{r}_k \right) + \ldots + \sum_{i_1<i_2<\ldots<i_N} u_N \left(\vec{r}_{i_1}, \vec{r}_{i_2} \ldots \vec{r}_{i_N} \right). \quad (2)$$

Jastrow's two-body correlations are contained in the function u_2; their importance for the ground-state energy, as shown by research on helium, are about 80% of the experimental results. The reason for this disagreement with experiments can be the omission of functions u_n ($n > 3$). Feenberg and Campbell analysed the general properties of functions u_n[4,5]. Woo, Campbell and Feenberg studied the influence of triplet function u_3 on the ground and excited states. Campbell[4] and later Schmidt et al.[6] found that the influence of triplet Feenberg effect on the ground-state is about 10%. Using the Monte Carlo method Woo and Coldwell[3] determined the influence of triplet Feenberg function in a two-dimensional model of the liquid ^{4}He; they stated that the contribution of the triplet Feenberg function to the ground-state was about 18%. Later it has been found[7] that in the spectrum of elementary excitations in liquid ^{4}He the triplet functions do not significantly improve the convolution approximation inclusively second order in the Brillouin--Wigner perturbation theory.

Correlations of the fourth and higher orders have not been studied so far. However, there are systems where correlations of the fourth and higher orders are not present at all. Those are three-body systems. Consequently a three-body system is the simplest possible system which, in addition to Jastrow's correlations, contains exclusively triplet correlations. For the three-body system Feenberg's exact function of the ground-state has the following form

$$\psi_3 (1, 2, 3) = \exp\left\{ -\frac{1}{2} \sum_{i,j}^{3} u_2 (\vec{r_i}, \vec{r_j}) - \frac{1}{6} \sum_{i,j,k}^{3} u_3 (\vec{r_i}, \vec{r_j}, \vec{r_k}) \right\}. \qquad (3)$$

In this paper equation (3) is applied to the ground-state of ^{4}He trimer. Let us note that ^{4}He trimer has been previously studied[8-14] in two (2D) and three dimensions (3D) but not on the basis of the relation (3).

Function u_2 in a system with a finite number of particles has a long-range part u_{lr}, besides the short-range part u_{sr}. The short-range part u_{sr} is already known from the many-body system theory. For a system containing several atoms the long-range part u_{lr} must increase monotonically as the system should be stable. This type of two-body function was first applied by Ljolje[15] and it has the following form

$$u_2 = u_{sr} + u_{lr}. \qquad (4)$$

In this paper we chose

$$u_{sr} = (a/r)^\beta \qquad (4'a)$$

which is a well known form of the function u_2 in many-body systems[16] and

$$u_{lr} = s \cdot r \qquad (4'b)$$

where a, β and s are variational parameters.

In the literature one finds several forms for the function u_3[1-3,6] related to correlations in many particles systems. In this paper we derive one form for the function u_3 and apply it to the ground-state of the ^{4}He trimer in 2D and 3D together with the function (4) (Sec. 2). Numerical analysis and discussion are presented in Section 3.

2. Formalism

A. Explicit form of u_3

Apart from being real, symmetric in arguments and invariant in terms of space inversion and translation, function u_3 should also be unique. Here uniqueness means that u_3 should not contain elements which are sums of u_2 terms. A simple form satisfying the above conditions is

$$u_3 (\vec{r}_1, \vec{r}_2, \vec{r}_3) \sim \frac{1}{f(r_{12}) + f(r_{13}) + f(r_{23})} \qquad (5)$$

were f is any function of interatomic distances. The following procedure may be followed to determine one form of the function f. There are such distributions of particles for which all arguments are equal, i. e. $r_{12} = r_{13} = r_{23} = d$. Those are configurations in which atoms are situated on the vertices of an equilateral triangle. Equation (5) in that case has the following form

$$u_3 (d, d, d) \sim \frac{1}{f(d)}. \qquad (6)$$

Function u_3 should furthermore be such that it becomes zero if any particle from its argument is far enough away (e. g. if that is particle 1, then $r_{12}, r_{13} \gg d_0$, where d_0 is the distance of the potential energy minimum). It is relatively large only when all the three prticles are close to each other. If we assume all the three particles far enough apart, the function u_3 should tend to zero. However, the same effect on physical quantities is obtained if we assume that u_3 in that case decomposes into the sum of two-body functions u_{sr}. Then, namely, we only change the factor of normalization in the function ψ_3 since the function ψ_3 contains already such terms in its exponent. Relation (6) becomes i. e.

$$1/f(d) \sim u_{sr}(d) + u_{sr}(d) + u_{sr}(d) \sim u_{sr}(d)$$
$$f(d) = u_{sr}^{-1}(d).$$

Expression (5) for a three-body function then becomes

$$u_3 (r_{12}, r_{23}, r_{31}) \sim \frac{1}{u_{sr}^{-1}(r_{12}) + u_{sr}^{-1}(r_{13}) + u_{sr}^{-1}(r_{23})} =$$
$$= A \frac{u_{sr}(r_{12}) u_{sr}(r_{23}) u_{sr}(r_{31})}{u_{sr}(r_{12}) u_{sr}(r_{13}) + (2; 1, 3) + (3; 1, 2)}, \qquad (7)$$

where A is a constant. Relation (7) can be generalized

$$u_3 (r_{12}, r_{13}, r_{23}) \sim \frac{\varphi(r_{12}) \varphi(r_{13}) \varphi(r_{23})}{\varphi(r_{12}) \varphi(r_{13}) + (2; 1, 3) + (3; 1, 2)}, \qquad (8)$$

where the function φ can be taken as a variational two-body function.

B. Application to trimer ^4He

The binding energy of the ^4He trimer can be determined on the basis of the variational principle

$$E < \langle \psi_3 |H| \psi_3 \rangle / \langle \psi_3 / \psi_3 \rangle, \tag{9}$$

where ψ_3 is the wave function (3) and the Hamiltonian

$$H = - \sum_{i}^{3} \frac{\hbar^2}{2m} \Delta_i + \frac{1}{2} \sum_{i,j}^{3} V(r_{ij}). \tag{10}$$

Using the properties of symmetry, the expression (9) can be written as follows

$$E = E_{2p} + E_{2k} + E_{k23} + E_{k3}. \tag{11}$$

E_{2p} and E_{2k} are potential and kinetic energies contained in the Jastrow's approximation; E_{k23} is kinetic energy due to *mixing* the Jastrow's and triplet Feenberg's correlations, and E_{k3} is the kinetic energy produced by the presence of triplet functions. Explicit forms of these expressions are

$$E_{2p} = \frac{1}{I_3} \cdot 3 \int \psi_3^2(1,2,3)\, V(1,2)\, d\vec{r}_{123}, \tag{12}$$

$$E_{2k} = \frac{1}{I_3} \cdot 3 \cdot 2 \cdot \left(-\frac{\hbar^2}{2m}\right) \int \psi_3^2(1,2,3) \left\{ u'_{12} u'_{13} \frac{\vec{r}_{12}\, \vec{r}_{13}}{r_{12} \cdot r_{13}} + \right.$$
$$\left. + u'^2_{12} - \left(u''_{12} + u'_{12} \frac{2}{r_{12}} \right) \right\} d\vec{r}_{123}, \tag{12'}$$

$$E_{k23} = \frac{1}{I_3} 3 \cdot 2 \cdot 2 \cdot \left(-\frac{\hbar^2}{2m}\right) \int \psi_3^2(1,2,3) \left\{ u'_{12} \frac{\partial u_3}{\partial r_{12}} + u'_{12} \frac{\partial u_3}{\partial r_{13}} \frac{\vec{r}_{12} \cdot \vec{r}_{13}}{r_{12} \cdot r_{13}} \right\} d\vec{r}_{123} \tag{13}$$

$$E_{k3} = \frac{1}{I_3} \cdot 3 \cdot 2 \cdot \left(-\frac{\hbar^2}{2m}\right) \int \psi_3^2(1,2,3) \left\{ \left(\frac{\partial u_3}{\partial r_{12}} \right)^2 + \frac{\partial u_3}{\partial r_{12}} \frac{\partial u_3}{\partial r_{13}} \frac{\vec{r}_{12} \cdot \vec{r}_{13}}{r_{12} \cdot r_{13}} - \right.$$
$$\left. - \frac{\partial^2 u_3}{\partial r_{12}} - \frac{\partial^2 u_3}{\partial r_{12}\, \partial r_{13}} \frac{\vec{r}_{12} \cdot \vec{r}_{13}}{r_{12} \cdot r_{13}} - \frac{\partial u_3}{\partial r_{12}} \frac{2}{r_{12}} \right\} d\vec{r}_{123} \tag{14}$$

The following notations are introduced

$$I_3 = \int \psi_3^2(1,2,3)\, d\vec{r}_{123}$$

$$u'_{ij} = \frac{du_2}{dr_{ij}}, \quad u''_{ij} = \frac{d^2 u_2}{dr_{ij}^2}. \tag{15}$$

Introducing the coordinates $\vec{x} = \vec{r_1} - \vec{r_2}$, $\vec{y} = \vec{r_1} - \vec{r_3}$ and $\vec{R} = (\vec{r_1} + \vec{r_2} + \vec{r_3})/3$ into expressions (12)—(15) and integrating, first over the coordinates of the center of mass $\vec{R}$, then over all angles except the angle between vectors $\vec{x}$ and $\vec{y}$ (angle ϑ); nine-fold integrals are reduced to the three-fold ones:

$$E_{2p} = \frac{1}{I} \cdot 3 \int_0^\infty dx \cdot x^2 \int_0^\infty dy \cdot y^2 \int_0^\pi d\vartheta \sin \vartheta \, V(x) \, \psi_3^2 \, (x, y, |\vec{x} - \vec{y}|), \quad (16)$$

$$E_{2k} = -\frac{1}{I} \cdot 3 \cdot 2 \left(-\frac{\hbar^2}{2m} \right) \int_0^\infty dx \cdot x^2 \int_0^\infty dy \cdot y^2 \int_0^\pi d\vartheta \sin \vartheta \left\{ u_x'^2 + \right.$$

$$\left. + u_x' u_y' \cos \vartheta - \left(u_x'' + u_x' \cdot \frac{2}{x} \right) \right\} \psi_3^2(x, y, |\vec{x} - \vec{y}|), \quad (17)$$

$$E_{k23} = \frac{1}{I} 3 \cdot 2 \cdot 2 \left(-\frac{\hbar^2}{2m} \right) \int_0^\infty dx \cdot x^2 \int_0^\infty dy \cdot y^2 \int_0^\pi d\vartheta \sin \vartheta \, u_x' \cdot$$

$$\cdot \left(\frac{\partial u_3}{\partial x} + \frac{\partial u_3}{\partial y} \cos \vartheta \right) \psi_3^2 \, (x, y, |\vec{x} - \vec{y}|), \quad (18)$$

$$E_{k3} = \frac{1}{I} 3 \cdot 2 \cdot \left(-\frac{\hbar^2}{2m} \right) \int_0^\infty dx \cdot x^2 \int_0^\infty dy \cdot y^2 \int_0^\pi d\vartheta \sin \vartheta \cdot \left\{ \left(\frac{\partial u_3}{\partial x} \right)^2 + \right.$$

$$\left. + \frac{\partial u_3}{\partial x} \frac{\partial u_3}{\partial y} \cos \vartheta - \frac{\partial^2 u_3}{\partial x^2} - \frac{\partial^2 u_3}{\partial x \partial y} \cos \vartheta - \frac{\partial u_3}{\partial x} \frac{2}{x} \right\} \psi_3^2 \, (x, y, |\vec{x} - \vec{y}|), \quad (19)$$

$$I = \int_0^\infty dx \cdot x^2 \int_0^\infty dy \cdot y^2 \int_0^\pi d\vartheta \sin \vartheta \, \psi_3^2 \, (x, y, |\vec{x} - \vec{y}|). \quad (20)$$

In all expressions for energies a factor $8\pi^2 \Omega$ is reduced in the numerators and denominators; the same factor was omitted in relation (20).

Expression (11) with the terms as in relations (16)—(20) can be integrated numerically. In order to achieve satisfactory accuracy a great deal of compute-time should be spent. In same papers, e. g. in Ref. 14, the three-dimensional integrals are reduced to one-dimensional by taking into account only some atom configurations; in Ref. 14 the atoms were assumed to be in the vertices of an equilateral triangle and having only such configurations. As this case leads to more general conclusions it is considered also in this paper (for two-body correlations). Thus, substituting $y = x$ and $\vartheta = \pi/3$ from (16), (17) and (20) it follows that the energy, for particle configurations corresponding to an equilateral triangle, is equal to

$$\varepsilon = \varepsilon_k + \varepsilon_p, \quad (21)$$

where

$$\varepsilon_k = \frac{1}{I_0} \, 2 \cdot \left(-\frac{\hbar^2}{2m}\right) \int\limits_0^\infty dx \cdot x^4 \, e^{-6u(x)} \cdot \left\{\frac{3}{2} u'(x) - u''(x) - u'(x) \cdot \frac{2}{x}\right\}, \quad (22)$$

$$\varepsilon_p = \frac{1}{I_0} \int\limits_0^\infty dx \cdot x^4 \, e^{-6u(x)} \, V(x), \quad (22')$$

$$I_0 = \int\limits_0^\infty dx \cdot x^4 \, e^{-6u(x)}. \quad (23)$$

3. *Numerical calculation and discussion*

In our calculations we shall use the Lennard-Jones (LJ) (12—6) potential

$$V(r) = 4 \, \varepsilon \left\{\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right\}, \quad (24)$$

with de Boer-Michels parameters $\sigma = 2.556 \times 10^{-10}$ m and $\varepsilon = 14.077 \cdot 10^{-23}$ J. Values of variational parameters α and β, which appear in the two-body function, have been determined earlier. Thus we chose $\beta = 5$ as in the many-particle system theory[15]. As the trimer ^{4}He was considered, we used the value $\alpha = 2.58 \times 10^{-10}$ m, as in case of ^{4}He dimer[16]. Thus the parameter s in the two-body function and the parameter A in the three-body function were used to minimize the energy.

One-fold integrals in relations (21)—(23) were computed using the Gauss quadrature formula with 32 points. The same algorithm, applied successively three times, was used also for the computation of the three-fold integrals (16)——(20). In quantum systems having large quantum effects the kinetic energy is big and close to potential energy; the cancellation between kinetic and potential energies renders the binding energy very small. A satisfactory accuracy was achieved, in this case, by dividing the integration domain into a large number of sub--domains and by applying the same procedure to each sub-domain. Numerical analysis was performed for two-dimensional (2D) and three-dimensional (3D) model.

Table I presents the results of computations for two-body correlations (2BC) in a model where atoms are in the vertices of an equilateral triangle. Expressions (21)—(23) are written for the case of 3D. The upper bound of the energy minima is obtained for $s = 0.21 \times 10^{10}$ m^{-1} with energy $\varepsilon = 0.843522 \times 10^{-23}$ J. This number compared with the variational calculation of energy $\varepsilon = -0.0869 \times 10^{-23}$ J (from Ref. 10), shows that the approximation of equal interatomic distances is not good enough (gives values from the lower side). It should be simply concluded that even considering the »best« position of particles (vertices of an equilateral triangle) the decrease in the potential energy is greater than the increase in the kinetic energy caused by the limitation of motion.

TABLE 1.

s	I	ε_p	ε_k	ε	
0.03	126696.27	−0.020862	0.011484	−0.009375	
0.04	29920.48	−0.061860	0.035814	−0.026046	
0.05	9717.661	−0.136198	0.082224	−0.053973	
0.06	3851.645	−0.249492	0.156126	−0.087372	
0.07	1747.79	−0.404004	0.260916	−0.143088	
0.08	874.082	−0.599938	0.398226	−0.201159	
0.09	470.1231	−0.833586	0.558314	−0.265269	
0.10	267.4654	−1.103574	0.770526	−0.333045	
0.11	159.0885	−1.405872	1.003608	−0.402264	
0.12	98.08921	−1.736886	1.265988	−0.470898	
0.13	62.29366	−2.093130	1.555942	−0.537186	3D
0.14	40.5464	−2.471340	1.871724	−0.599616	
0.15	26.95251	−2.868528	2.211618	−0.656907	
0.16	18.23779	−3.281988	2.574012	−0.707976	
0.17	12.53301	−3.709308	2.957376	−0.750193	
0.18	8.729568	−4.148340	3.360312	−0.788028	
0.19	6.152915	−4.597170	3.781523	−0.815649	
0.20	4.382629	−5.054118	4.219830	−0.834285	
0.21	3.151093	−5.517684	4.676162	−0.843522	
0.22	2.284788	−5.98654	5.143524	−0.843015	
0.23	1.669295	−6.459522	5.627038	−0.832485	
0.24	1.228055	−6.935586	6.123876	−0.811707	
0.26	0.676950	−7.893343	7.154646	−0.738696	
0.30	0.218570	−9.811122	9.347460	−0.463662	
0.34	0.075189	−11.70298	11.689518	−0.01346	
0.38	0.027164	−13.54438	14.157354	0.612975	
0.42	0.010206	−15.31843	16.733472	1.415042	

Energy of LJ (12, 6) ⁴He trimer in the approximation of the averaging over atomic positions when equilateral triangles are formed; s — parameter in 10^{10} m^{-1}, I — normalization integral; ε_p, ε_k and ε are the potential, kinetic and total energy measured in 10^{-23} J.

TABLE 2.

A	s	I	E_{2p}	E_{2k}	E_2	E_{k23}	E_{k3}	E	
	0.06	1527.728	−1.35392	1.20767	−0.14625				
	0.07	744.692	−1.70097	1.54981	−0.151159				2BC
	0.08	391.256	−2.05725	1.91467	−0.14258				
0.5	0.06864	816.343	−1.64817	1.49698	−0.15119	−0.001624	0.00525	−0.14756	
0.2	"	816.819	−1.6511	1.49987	−0.15123	−0.00068	0.002136	−0.14977	3BC
0.1	"	816.978	−1.65211	1.50085	−0.15127	−0.00036	0.001074	−0.15055	
0.05	"	817.058	−1.65261	1.50133	−0.15128	−0.00015	0.00054	−0.15069	

Energy of the LJ (12, 6) ⁴He trimer in two dimensions as a function of the variation parameters A and s; s is measured in 10^{10} m^{-1}; I — normalization integral; E_{2p}, E_{2k}, E_2 are the potential, kinetic and total energy which are contained also in the Jastrow's correlations; E_{k23} and E_{k3} are the kinetic energies due to two-triplet correlations and due to triplet correlations; E is total energy. All energies are measured in 10^{-23} J.

Table 2 summarizes the results of the entire problem in 2D in terms of the relations (16)—(20). The first part of Table 2 related to 2BC, and the second which, apart from 2BC, contains the triplet effect is denoted as 3BC. From relations (16)—

—(20) one passes to the two-dimensional case upon substitution $x^2 y^2 \to xy$, $2/x \to \to 1/x$ and $\sin \vartheta \to 1$. The best values for 2BC, after interpolation, are: $s = 0.06864 \cdot \cdot 10^{10}$ m^{-1} and the corresponding upper bound of the energy minimum $E_2 = = -0.151286 \cdot 10^{-23}$ J. Triplet Feenberg function, as shown in the second part of Table 2, doesn't lower the energy minimum; the best value of the energy is obtained for $A \to 0$ i. e. $E \to E_2$. Three body correlation function in 2D doesn't improve the energy in the right direction. Cabral and Bruch[11] found that this energy is $E_2 = -0.155185 \cdot 10^{-23}$ J using the wave function $\Phi(r)\,\Phi(s)\,\Phi(t)$, where Φ is the numerical solution of two-dimensional Schrödinger's equation for two particles. Lim et al.[12,13] carried an extensive study of these systems within 2BC using various computation techniques. Introducing the parameter $\eta = \hbar^2/(m\varepsilon\sigma^2)$, where m is the mass, ε and σ are parameters of the LJ (12, 6) potential, it was possible to study the binding energy dependence on mass and parameters of the potential. For the LJ potential with de Boer-Michels parameters and mass of ^{4}He we obtain $\eta = 0.182166$. Interpolating the results from Ref. 12 we get the binding energy $\varepsilon = -0.15199 \times 10^{-23}$ J in 2D. Comparison of all these results confirms the reliability of Ljolje's wave function (4), which although simple, yields the result only a few percent less reliable than the numerical solution (for 2BC).

The computation of the exact expressions in 3D shows that the upper bound of the energy minimum is obtained for $s = 0.12 \times 10^{10}$ m^{-1} and this is $E_{2BC} = = -0.36218 \times 10^{-24}$ J for 2BC, and $s = 0.12 \times 10^{10}$ m^{-1} and $A \to 0$, $E_{3BC} \to \to E_{2BC}$ for 3BC. The influence of the triplet function described by function u_3, is not in the right direction in 3D as well. The minimum energy is obtained after making the effect of triplet Feenberg function tend to zero. On the other hand the trimer energy in 3D is greater than its energy in 2D. It means that the trimer is more tightly bound in 2D than in 3D. Dimer ^{4}He behaves similarly (bound in 2D and not in 3D, at least for two-body functions of the Ljolje's type)[17]. This conclusion is confirmed by the discussion in Ref. 11. However, in a many particle system we have an inverse situation: the binding energy per particle in liquid ^{4}He in 3D is greater than the corresponding binding energy in 2D[3,18]. Qualitative explanation of these results can be given in the following way. Generally, the limitation of motion in 2D is effectively in favour of the potential energy. However, when a many-particle system is considered, each particle has its neighbourhood which is not the same in 2D as in 3D. So for example one atom has about 6 neighbours in a plane, and about 12 neighbours in space. Each neighbouring atom increases the average binding energy. As the number of an atom's neighbours in a plane is different from the one in space and as it is favour of atom in space, the limitation effect in 2D will be overshadowed by a greater number of neighbouring atoms in 3D for a given number of neighbours. According to the possible distribution of the particles and the result from Ref. 12 it follows that four atoms are the first structure where this is realized.

The results obtained here for trimer ^{4}He in 3D is not in agreement with the corresponding result from Ref. 12 by about a factor of 2. So we took a better form of u_2 function[10]

$$u_2 = \begin{cases} u(r)/r, & r < d \\ \dfrac{A}{r^{1/2}}\{\exp(-\gamma r) + B \exp(-\delta r)\}, & r > d \end{cases} \qquad (25)$$

where u is a numerical solution of the equation

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + [V(r) - e]\,u = 0 \tag{26}$$

and we found that

$$E_{2BC} = -\,0.0789 \cdot 10^{-23}\,J$$

for $e = -0.13804 \cdot 10^{-23}\,J$

$A = 2.371417$

$B = -0.715353$

$\gamma = 0.07 \times 10^{10}\,m^{-1}$

$\delta = 0.43 \times 10^{10}\,m^{-1}$

$d = 5.48 \times 10^{-10}\,m.$

To demonstrate the effects of other forms of the function u_3 on the trimer ^{4}He energy, we employed

1) Woo's function

$$u_{3,1} = \left\{\frac{C}{R}\right\}^n, \quad R = \sqrt{r_{12}^2 + r_{13}^2 + r_{23}^2} \tag{27}$$

2) $u_{3,2} = D\,e^{-E(r_{12}+r_{13}+r_{23})}$ \tag{28}

3) $u_{3,3} = u_{3,1} + F \cdot R$ \tag{29}

4) $u_{3,4} = u_{3,1} + F \cdot R_p; \quad R_p = \{(r_{12} - t)\,(r_{13} - t)\,(r_{23} - t)\}^n$ \tag{30}

5) $u_{3,5} = u_{3,1} + Q \cdot (r_{12} \cdot r_{13} \cdot r_{23}).$ \tag{31}

All these functions have been used in 2D case. The results showed that the energy minima were produced if triplet function tends to zero.

Finally we can conclude that triplet Feenberg's effects are not significant in this system. This result can be explained if we take into account that triplet effects are the effects of the short range and that the particles are far enough apart. Namely, the probability to find two particles at the distance x in ^{4}He trimer (in 2D) is

$$w(x) = \frac{x \cdot \int\limits_0^\infty dy \cdot y \int\limits_0^\pi d\varphi\,\psi_3^2\,(x,y,|\vec{x}-\vec{y}|)}{\int\limits_0^\infty dx \cdot x \int\limits_0^\infty dy \cdot y \int\limits_0^\pi d\varphi\,\psi_3^2\,(x,y,|\vec{x}-\vec{y}|)} \cdot$$

This function has been numerically derived and it is presented in Fig. 1; its maximum is around $6.7 \cdot 10^{-10}$m.
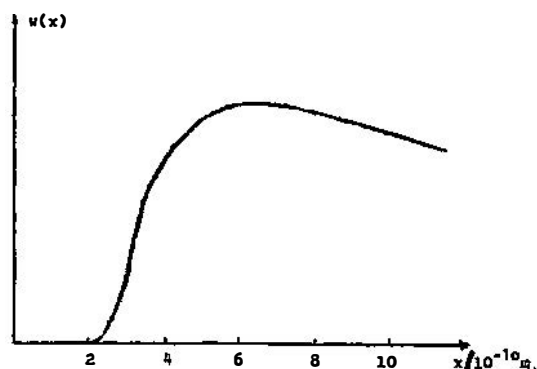

Fig. 1. The probability of finding two particles at distance x.

The numerical analysis was performed on computers: UNIVAC 1100 University Computational Center, Zagreb and PDP 11/34 at the Department of Civil Engineering, University of Split.

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O TRIPLETNIM KORELACIONIM EFEKTIMA U TRIMERU ^{4}He

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U radu je određen izraz za tripletnu Feenbergovu funkciju u koordinatnom prostoru. Koristeći ovaj rezultat i varijacioni princip određena je energija trimera ^{4}He. Za potencijal međudjelovanja između atoma uzet je Lennard-Jones (12, 6) potencijal. Pokazano je da je u ovom sistemu utjecaj tripletnih korelacija zanemariv. Zaključak je izveden na temelju razmatranja više oblika probnih funkcija.