

# DIFFERENT POTENTIALS AND MULTIPLE CORRELATIONS IN THE ATOMIC SPHERE MODEL OF LIQUID $^4\text{He}$

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It has been shown that the two-body correlation function which minimizes energy has, for small interatomic distances, the form  $u_2 \sim -\ln r^2 + \left(\frac{\alpha}{r}\right)^5$ , in the low density limit in the approximation of the hard spheres. Furthermore it has been established that in the same limit the Wu-Feenberg-Ljolje two-body function yields minimum energy for the Maitland-Smith potential and in comparison with Lennard-Jones potential is better for 9%. It has also been found out that the influence of the triplet correlations in this model is negligible, and that the three-particle potential gives a contribution greater than zero and smaller than 0.6% with regard to the two-body potential.

## 1. Introduction

The ground state of the liquid  $^4\text{He}$  has been intensively studied so far on the base of Feenberg's function:

$$\psi(1, 2, \dots, N) = e^{\frac{1}{2} \bar{U}(1, 2, \dots, N)} \quad (1)$$

where  $N$  is the number of atoms in the volume  $\Omega$ , and

$$\bar{U} = - \sum_{i < j} u_2(\vec{r}_i, \vec{r}_j) - \sum_{i < j < k} u_3(\vec{r}_i, \vec{r}_j, \vec{r}_k) - \dots \quad (2)$$

The functions  $u_i$  are real. Two-body correlations, so called Jastrow correlations, are described by the terms  $u_2$ , the triplet correlations by  $u_3$  etc. For this purpose various techniques were used: the Monte Carlo method, molecular dynamics method, *hypernetted chain* and other *cluster* theories. Mainly all these methods belong to the category of the semi-free gas model (SFG) of the liquid  $^4\text{He}$ <sup>1)</sup>. In this model the two-body particle correlations at small distances are determined from the Ljolie's equation

$$\left( \frac{d u_2(r)}{dr} \right)^2 = \frac{m}{\hbar^2} V(r) \Big|_{r \rightarrow 0} \quad (3)$$

where  $V(r) \Big|_{r \rightarrow 0}$  is a two-body potential between the atoms at small interatomic distances. In the remaining space the particles move freely. For example, the solution of equation (3) for the Yntema-Schneider potential has the following form:

$$u_2(r) = B e^{-\frac{\gamma}{2}r} \quad (4)$$

where for the atoms of  $^4\text{He}$   $B = 359$  and  $\gamma = 4.717 \cdot 10^{-10} \text{ m}^{-1}$ . For the Lennard-Jones potential the solution has the form

$$u_2(r) = \left( \frac{a}{r} \right)^5 \quad (4')$$

where  $a = 2.523 \cdot 10^{-10} \text{ m}$ .

Only functions  $u_2$  describing at the same time the long-range correlations do not belong to the SFG model. They are according to Ref. 2 the functions whose asymptotic behaviour for large  $r$  is  $u_2 \sim r^{-2}$ .

Originally in Ref. 1 the semi-free gas model was combined with the approximation of hard spheres which was used to reduce the  $n$ -dimensional integrals ( $n \geq 1$ ) to one- and three-dimensional ones. With this approximation the SFG models gives, in a simple analytic manner, the quantitative behaviour of the ground state of the liquid  $^4\text{He}$ .

During the past few years numerous new potentials have been used to describe the interaction between the helium atoms. In addition, the influence of many-body correlations, particularly the triplet one, has been intensively studied.

The object of this paper is to analyze the influence of various potentials and many-body correlations of the semi-free gas model on the ground-state of the liquid helium in the approximation of hard spheres.

## 2. Energy of the ground state in the approximations of hard spheres

Consider the system of  $N$  atoms of  $^4\text{He}$  in volume  $\Omega$ . The ground-state energy  $E_0$  satisfies the relation

$$E_0 < E = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \quad (5)$$

where,

$$H = T + V,$$

$$T = -\frac{\hbar^2}{2m} \sum_i^N \Delta_i,$$

$$V = V_2 + V_3.$$

Potentials  $V_2$  and  $V_3$  are two-body and three-body potentials of interaction and are determined in the Appendix.

Using the relation

$$\int \psi \Delta \psi \, d\tau = - \int \nabla \psi \cdot \nabla \psi \, d\tau \quad (6)$$

satisfied by functions  $\psi$  because of their asymptotic behaviour, it is possible to form three forms of the operator of the kinetic energy

$$A \rightarrow \int \psi \Delta \psi \, d\tau,$$

$$B \rightarrow - \int \nabla \psi \cdot \nabla \psi \, d\tau,$$

$$C \rightarrow \frac{1}{2} \int (\psi \Delta \psi - \nabla \psi \cdot \nabla \psi) \, d\tau.$$

All the three forms should yield the same results if the computation is correct. Taking into account the terms with  $u_2$  and  $u_3$  functions of the Feenberg's function, in case  $B$  we have

$$\frac{E_B}{N} = T_2 + T_{23} + T_{33} + V_{p2} + V_{p3} \quad (7)$$

where

$$\begin{aligned} T_2 = & \frac{1}{I_N} (N-1) \frac{\hbar^2}{2m} \int |\psi_3(1, 2, \dots, N)|^2 \left[ \frac{d u_2(r_{12})}{d r_{12}} \right]^2 d\vec{r}_1 \dots d\vec{r}_N + \\ & + \frac{1}{I_N} (N-1) (N-2) \frac{\hbar^2}{2m} \int |\psi_3(1, 2, \dots, N)|^2 \frac{d u_2(r_{12})}{d r_{12}} \frac{d u_2(r_{13})}{d r_{13}} \frac{\vec{r}_{12} \vec{r}_{13}}{r_{12} r_{13}} \cdot d\vec{r}_1 \dots d\vec{r}_N, \end{aligned} \quad (8)$$

$$\begin{aligned} T_{23} = & \frac{1}{I_N} 2(N-1) (N-2) \frac{\hbar^2}{2m} \int |\psi_3(1, 2, \dots, N)|^2 \left[ \frac{d u_2(r_{12})}{d r_{12}} \frac{\partial u_3(1, 2, 3)}{\partial r_{12}} + \right. \\ & + \left. \frac{d u_2(r_{12})}{d r_{12}} \frac{\partial u_3(1, 2, 3)}{\partial r_{13}} \frac{\vec{r}_{12} \vec{r}_{13}}{r_{12} r_{13}} \right] d\vec{r}_1 \dots d\vec{r}_N + \frac{1}{I_N} 2(N-1) (N-2) (N-3) \cdot \\ & \cdot \frac{\hbar^2}{2m} \int |\psi_3(1, 2, \dots, N)|^2 \frac{d u_2(r_{12})}{d r_{12}} \frac{\partial u_3(1, 3, 4)}{\partial r_{13}} \frac{\vec{r}_{12} \vec{r}_{13}}{r_{12} r_{13}} d\vec{r}_1 \dots d\vec{r}_N, \end{aligned} \quad (9)$$

$$\begin{aligned}
T_{33} = & \frac{1}{I_N} (N-1)(N-2) \frac{\hbar^2}{2m} \int |\psi_3(1, 2, \dots, N)|^2 \left[ \frac{\partial u_3(1, 2, 3)}{\partial r_{12}} \frac{\partial u_3(1, 2, 3)}{\partial r_{13}} \right. \\
& \cdot \frac{\vec{r}_{12} \vec{r}_{13}}{r_{12} r_{13}} + \left. \frac{\partial u_3(1, 2, 3)}{\partial r_{12}} \frac{\partial u_3(1, 2, 3)}{\partial r_{12}} \right] d\vec{r}_1 \dots d\vec{r}_N + \\
& + \frac{1}{I_N} (N-1)(N-2)(N-3) \frac{\hbar^2}{2m} \int |\psi_3(1, 2, \dots, N)|^2 \left[ \frac{\partial u_3(1, 2, 3)}{\partial r_{12}} \frac{\partial u_3(1, 2, 4)}{\partial r_{12}} + \right. \\
& + 2 \frac{\partial u_3(1, 2, 3)}{\partial r_{12}} \frac{\partial u_3(1, 2, 4)}{\partial r_{14}} \frac{\vec{r}_{12} \vec{r}_{14}}{r_{12} r_{14}} + \\
& + \left. \frac{\partial u_3(1, 2, 3)}{\partial r_{13}} \frac{\partial u_3(1, 2, 4)}{\partial r_{14}} \frac{\vec{r}_{13} \vec{r}_{14}}{r_{13} r_{14}} \right] d\vec{r}_1 \dots d\vec{r}_N + \\
& + \frac{1}{I_N} 4(N-1)(N-2)(N-3)(N-4) \frac{\hbar^2}{2m} \int |\psi_3(1, 2, \dots, N)|^2 \cdot \\
& \cdot \frac{\partial u_3(1, 2, 3)}{\partial r_{12}} \frac{\partial u_3(1, 4, 5)}{\partial r_{14}} \frac{\vec{r}_{12} \vec{r}_{14}}{r_{12} r_{14}} d\vec{r}_1 \dots d\vec{r}_N, \quad (10)
\end{aligned}$$

$$V_{p2} = \frac{1}{2I_N} (N-1) \int |\psi_3(1, 2, \dots, N)|^2 V_2(r_{12}) d\vec{r}_1 \dots d\vec{r}_N, \quad (11)$$

$$V_{p3} = \frac{1}{6I_N} (N-1)(N-2) \int |\psi_3(1, 2, \dots, N)|^2 V_3(\vec{r}_1, \vec{r}_2, \vec{r}_3) d\vec{r}_1 \dots d\vec{r}_N, \quad (12)$$

$$I_N = \langle \psi_3 | \psi_3 \rangle, \quad (13)$$

$$\psi_3 = e^{-\frac{1}{2} \sum_{i,j} u_3(\vec{r}_i, \vec{r}_j) - \frac{1}{6} \sum_{i,j,k} u_3(\vec{r}_i, \vec{r}_j, \vec{r}_k)}. \quad (14)$$

In the approximation of hard spheres<sup>1,3)</sup> the expression for energy, after taking the relative coordinates, has the following form

$$\frac{E_B}{N} = \varrho I_{1B} + \varrho^2 I_{2B} + \varrho^3 I_{3B} + \varrho^4 I_{4B} \quad (15)$$

where

$$I_{1B} = 2\pi \int_0^\infty e^{-2u_2(x)} \left( \frac{\hbar^2}{m} u_2'^2 - V_2(x) \right) x^2 dx, \quad (16)$$



$$\begin{aligned}
I_{2B} = & 4\pi^2 \int_0^\infty \int_0^\infty \int_{-1}^1 e^{-2u_2(x) - 2u_2(y) - 2u_2(|\vec{x} - \vec{y}|) - 2u_3(x, y, |\vec{x} - \vec{y}|)} \\
& \cdot \left\{ \frac{\hbar^2}{m} \left[ u'_2(x) u'_2(y) t + 2 u'_2(x) \left( \frac{\partial u_3}{\partial x} + \frac{\partial u_3}{\partial y} t \right) + \left[ \left( \frac{\partial u_3}{\partial x} \right)^2 + \frac{\partial u_3}{\partial x} \frac{\partial u_3}{\partial y} t \right] \right\} + \right. \\
& \left. + \frac{1}{3} V_3(x, y, |\vec{x} - \vec{y}|) \right\} x^2 y^2 dx dy dt. \quad (17)
\end{aligned}$$

With regard to the use of the approximation of hard atomic spheres and the object of this paper, we shall consider only the first two terms of the expansion (15). Therefore we do not state the explicit forms for  $I_{3B}$  and  $I_{4B}$ . The other two forms for the operators of kinetic energy lead to the expansion (up to the second order)

$$\frac{E_A}{N} = \varrho I_{1A} + \varrho^2 I_{2A}, \quad (18)$$

$$\frac{E_C}{N} = \varrho I_{1C} - \varrho^2 I_{2C} \quad (19)$$

where

$$I_{1A} = 2\pi \int_0^\infty e^{-2u_2(x)} \left\{ \frac{\hbar^2}{m} \left[ u''_2 + \frac{2}{x} u'_2 - u_2'' \right] + V_2(x) \right\} x^2 dx, \quad (20)$$

$$\begin{aligned}
I_{2A} = & 4\pi^2 \int_0^\infty \int_0^\infty \int_{-1}^1 e^{-2u_2(x) - 2u_2(y) - 2u_2(|\vec{x} - \vec{y}|) - 2u_3(x, y, |\vec{x} - \vec{y}|)} \\
& \cdot \left\{ -\frac{\hbar^2}{m} \left[ u'_2(x) u'_2(y) t + 2 u'_2(x) \left( \frac{\partial u_3}{\partial x} + \frac{\partial u_3}{\partial y} t \right) + \frac{\partial^2 u_3}{\partial x^2} + \frac{\partial^2 u_3}{\partial x \partial y} t + \frac{2}{x} \frac{\partial u_3}{\partial x} - \right. \right. \\
& \left. \left. - \frac{\partial u_3}{\partial x} \frac{\partial u_3}{\partial y} t - \left( \frac{\partial u_3}{\partial x} \right)^2 \right] + \frac{1}{3} V_3(x, y, |\vec{x} - \vec{y}|) \right\} x^2 y^2 dx dy dt, \quad (21)
\end{aligned}$$

$$I_{1C} = 2\pi \int_0^\infty e^{-2u_2(x)} \left[ \frac{\hbar^2}{m} (u''_2 + \frac{2}{x} u'_2) + V_2(x) \right] x^2 dx, \quad (22)$$

$$\begin{aligned}
I_{2C} = & 4\pi^2 \frac{1}{3} \int_0^\infty \int_0^\infty \int_{-1}^1 e^{-2u_2(x) - 2u_2(y) - 2u_2(|\vec{x} - \vec{y}|) - 2u_3(x, y, |\vec{x} - \vec{y}|)} \\
& \cdot V_3(x, y, |\vec{x} - \vec{y}|) x^2 y^2 dx dy dt. \quad (23)
\end{aligned}$$

It can be seen that three different operators for kinetic energy lead to different expressions for energy. This result is the consequence of the approximation we used.

In the low density limit the first term is dominant, so the computation includes only two-body correlations; the boundary condition, which they satisfy in the approximation of the SFG model, is:

$$4\pi \int_0^{\infty} dx x^2 (1 - e^{-2u_2(x)}) = \text{finite number.} \quad (24)$$

We can look for this function for which the expression

$$\frac{E[u_2]}{N} = \varrho I_1 \quad (25)$$

is extreme. It is shown that the respective functionals, where instead of  $I_1$  we have  $I_{1A}$ ,  $I_{1B}$  or  $I_{1C}$ , have the extreme for the functions  $u_2$  which are solutions of equation<sup>4)</sup>

$$u_2'' + \frac{2}{x} u_2' - u_2'^2 + \frac{m}{\hbar^2} (V_2 + 2\lambda) = 0. \quad (26)$$

$\lambda$  is the Lagrange multiplier for condition (24). Equation (26) in case of the Lennard-Jones potential in the region of small  $x$  has the general solution

$$u_2 = -\ln \left\{ C_1 x^{-\frac{1}{2}} \mathcal{Y}_{-\frac{1}{10}} \left[ -i \left( \frac{a}{x} \right)^5 \right] + C_2 x^{-\frac{1}{2}} N_{-\frac{1}{10}} \left[ -i \left( \frac{a}{x} \right)^5 \right] \right\} \quad (27)$$

where  $C_1$  and  $C_2$  are arbitrary constants, and  $\mathcal{Y}$ , and  $N$ , the respective Bessel functions. The asymptotic behaviour of the Bessel functions for large arguments is valid in the region of small values of  $x$ . By a suitable selection of the coefficients it is possible to satisfy the general correct behaviour of  $u_2$  so that the expression in braces is proportional to the Hankel function  $x^{1/2} H_0^{(2)}$ . Thus relation (27) becomes

$$u_2 = -\ln x^2 + \left( \frac{a}{x} \right)^5. \quad (28)$$

This expression represents a new result. Woo-Feenberg-Ljolje asymptotic function is not a solution of the problem of the extreme in the region of densities where the first term of expansion (15) is dominant.

The triplet correlations are described by function  $u_3$ . Their general property is that they decrease rapidly, when one of the arguments becomes large; they are significant only when all the three arguments are small. This is the property of, e. g. Woo-Coldwell<sup>5)</sup>

$$u_3 = \left( \frac{A}{R} \right)^B, \quad R = \sqrt{x^2 + y^2 + |\vec{x} - \vec{y}|^2} \quad (29)$$

as well as<sup>6)</sup>

$$u_3 = \frac{C}{\frac{1}{u_2(x)} - \frac{1}{u_2(y)} - \frac{1}{u_2(|\vec{x}-\vec{y}|)}} \quad (30)$$

$A$ ,  $B$  and  $C$  are parameters here.

The numerical analysis was performed first in the low density limit, where the first term is dominant for both forms of functions (4) and (4') and for different potentials. The results are presented in Table. The results show that function (4) yields smaller energies for all potentials and the Maitland-Smith potential has the minimum value.

TABLE

Potential	$\alpha$	$\beta$	$\varepsilon/\varrho$	$A$	$B$	$\varepsilon/\varrho$
	( $10^{-10}\text{m}$ )		( $10^{-23}\text{Jm}^3$ )	( $10^{-10}\text{m}$ )		( $10^{-23}\text{Jm}^3$ )
L—J	2.38	6.746	—5.578	4.879	363.45	—5.678
Y—S	2.465	6.17	—3.608	4.717	340.0	—3.757
B—McG	2.467	6.271	—3.179	4.764	360.87	—3.346
MDD-2	2.46	6.9	—5.602	4.757	363.29	—5.774
Beck	2.428	6.8	—5.495	4.819	364.15	—5.667
MS12G6	2.429	7.0	—6.045	4.809	362.90	—6.187
ESMMSV	2.45	6.84	—5.478	4.778	362.48	—5.647
Aziz	2.433	6.942	—5.754	4.8	367.09	—5.905

Energy per particle in the low density limit for different potentials and for the functions  $u_2$  taking form (4) and (4').

The computation of the influence of triplet correlations was performed by a numerical minimization of the energy expression which includes the first two terms in the series (15), where the three-body potential  $V_3$  is excluded from the integral. The Woo-Coldwell function (29) was taken as a trial function. It was found out that the energy minimum is obtained if the contribution of the triplet correlations tends to zero.

By a computation of the complete integral  $I_2$  it was found that the contribution of the three-body potential  $V_3$  is positive and that its contributions for experimental densities are under 0.6% compared with the Lennard-Jones two-body potential.

#### Acknowledgment

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#### APPENDIX

##### *Potentials of interaction of helium atoms*

There are several forms of potentials of interaction between helium atoms in literature:

## 1. Lennard-Jones (L-J)

$$V_2(r) = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] \quad (\text{A1})$$

$$\varepsilon = 14.108 \cdot 10^{-23} \text{ J}$$

$$\sigma = 2.556 \cdot 10^{-10} \text{ m.}$$

## 2. Yntema-Schneider (Y-S)

$$V_2(r) = \begin{cases} a e^{-\alpha r} - \frac{b}{r^6} - \frac{c}{r^8}, & r > r_0 \\ a e^{-\alpha r}, & r < r_0 \end{cases} \quad (\text{A2})$$

$$a = 1200 \cdot 10^{-19} \text{ J}$$

$$b = 1.24 \cdot 10^{-79} \text{ J} \cdot \text{m}^6$$

$$c = 1.89 \cdot 10^{-99} \text{ J} \cdot \text{m}^8$$

$$\alpha = 1/0.212 \cdot 10^{10} \text{ m}^{-1}$$

$$r_0 = 10^{-10} \text{ m.}$$

## 3. Bruch-McGee (B-McG)

$$V_2(r) = \begin{cases} \varepsilon \left[ B^2 e^{-\frac{2r}{a}} - 2B e^{-\frac{r}{a}} \right], & r < r_0 \\ -\frac{C_6}{r^6} - \frac{C_8}{r^8}, & r > r_0 \end{cases} \quad (\text{A3})$$

$$\varepsilon = 12.7687 \cdot 10^{-23} \text{ J}$$

$$a = 0.49413 \cdot 10^{-10} \text{ m}$$

$$C_6 = 9444.6969 \cdot 10^{-83} \text{ J} \cdot \text{m}^6$$

$$C_8 = 37174.172 \cdot 10^{-103} \text{ J} \cdot \text{m}^8$$

$$B = 455.674$$

$$r_0 = 3.6828 \cdot 10^{-10} \text{ m.}$$

## 4. Bruch-McGee (MDD-2)

$$V_2(r) = 10^{-23} V^*(r)$$

$$V^*(r) = \begin{cases} 2.74292 \cdot 10^6 \exp(-3.4573 r - 0.26206 r^2), & r < 0.8919 \cdot 10^{-10} \text{ m} \\ 14.839024 \{\exp[2C(1-\chi)] - 2 \exp[C(1-\chi)]\}, & 0.8919 \cdot 10^{-10} \text{ m} \leq r < 3.682 \cdot 10^{-10} \text{ m} \\ -10^4 (1.409907/r^6 + 3.819749/r^8), & 3.682 \cdot 10^{-10} \text{ m} \leq r \end{cases} \quad (\text{A4})$$

$$C = 6.127768$$

$$\chi = r/(3.0238 \cdot 10^{-10} \text{ m}).$$

## 5. Beck (B)

$$V_2(r) = A e^{-\alpha r - \beta r^6} - \frac{B}{(r^2 + a^2)^3} \left( 1 + \frac{2.709 + 3a^2}{r^2 + a^2} \right) \quad (\text{A5})$$

$$a = 0.675 \cdot 10^{-10} \text{ m}$$

$$\alpha = 4.390 \cdot 10^{10} \text{ m}^{-1}$$

$$A = 640.35937 \cdot 10^{-19} \text{ J}$$

$$\beta = 3.746 \cdot 10^{56} \text{ m}^{-6}$$

$$B = 1.392249 \cdot 10^{-19} \text{ J}.$$

## 6. Maitland-Smith (MS12G6)

$$V_2(r) = \varepsilon V^*(r)$$

$$V^*(r) = \frac{6}{n-6} \left( \frac{r_m}{r} \right)^n - \frac{n}{n-6} \left( \frac{r_m}{r} \right)^6 \quad (\text{A6})$$

$$n = 12 + 6 \left( \frac{r}{r_m} - 1 \right)$$

$$r_m = 2.967 \cdot 10^{-10} \text{ m}$$

$$\varepsilon = 15.04636 \cdot 10^{-23} \text{ J}$$

## 7. Farrar-Lee (ESMMSV)

$$V_2(r) = \varepsilon f \left( \frac{r}{r_m} \right)$$

$$\begin{aligned}
f(x) &= A \exp[-a(x-1)], & x < x_1 \\
&= \exp\{a_1 + (x-x_1)\{a_2 + (x-x_2)[a_3 + (x-x_1)a_4]\}\}, & x_1 < x < x_2 \\
&= \exp[-2\beta(x-1)] - 2 \exp[-\beta(x-1)], & x_2 < x < 1 \\
&= \exp[-2\beta'(x-1)] - 2 \exp[-\beta'(x-1)], & 1 < x < x_3 \\
&= b_1 + (x-x_3)\{b_2 + (x-x_4)[b_3 + (x-x_3)b_4]\}, & x_3 < x < x_4 \\
&= -C_6 x^{-6} - C_8 x^{-8} - C_{10} x^{-10}, & x_4 < x
\end{aligned}
\tag{A7}$$

$$C_n = D_n / \varepsilon r_m^n$$

$$\varepsilon = 14.590828 \cdot 10^{-23} \text{ J}$$

$$\beta = 6.475 \quad \beta' = 5.964$$

$$r_m = 2.97 \cdot 10^{-10} \text{ m}$$

$$A = 0.343 \quad a = 15.058$$

$$a_1 = 3.4469 \quad a_2 = -19.0218 \quad a_3 = -28.0670 \quad a_4 = -362.002$$

$$b_1 = -0.65 \quad b_2 = 1.4516 \quad b_3 = -4.02889 \quad b_4 = 4.51927$$

$$x_1 = 0.7 \quad x_2 = 0.84477 \quad x_3 = 1.15016 \quad x_4 = 1.5$$

$$D_6 = 1.4 \cdot 10^{-79} \text{ J} \cdot \text{m}^6$$

$$D_8 = 3.78 \cdot 10^{-99} \text{ J} \cdot \text{m}^8$$

$$D_{10} = 13.7 \cdot 10^{-119} \text{ J} \cdot \text{m}^{10}.$$

#### 8. Aziz and others (HFDHE2)

$$V_2(r) = \varepsilon V^*(r)$$

$$V^*(r) = A e^{-d \frac{r}{r_m}} - \left[ C_6 \left( \frac{r_m}{r} \right)^6 + C_8 \left( \frac{r_m}{r} \right)^8 + C_{10} \left( \frac{r_m}{r} \right)^{10} \right] F(r) \tag{A8}$$

$$F(r) = \begin{cases} e^{-\left(D \frac{r_m}{r} - 1\right)^2} & \frac{r}{r_m} < D \\ 1 & \frac{r}{r_m} > D \end{cases}$$

$$\varepsilon = 14.90832 \cdot 10^{-23} \text{ J}$$

$$D = 1.241314$$

$$r_n = 2.9673 \cdot 10^{-10} \text{ m}$$

$$C_6 = 1.3732412$$

$$A = 0.5448504 \cdot 10^6$$

$$C_8 = 0.4253785$$

$$\alpha = 13.353384$$

$$C_{10} = 0.178100.$$

All these potentials are presented in Figs. 1 and 2.

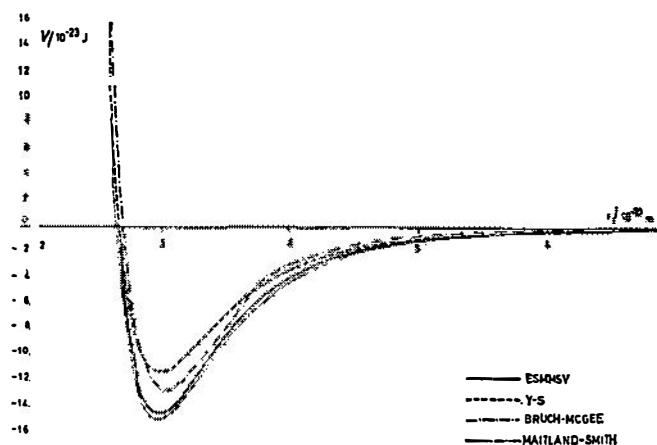


Fig. 1. Two-body potentials between helium atoms.

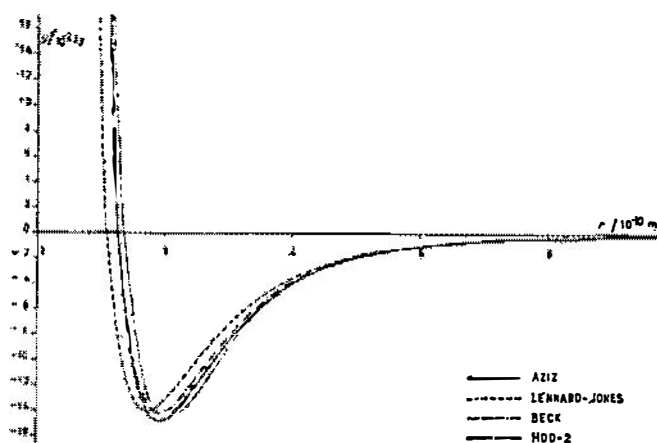


Fig. 2. Two-body potentials between helium atoms.

In literature there is a three-body potential of interaction between helium atoms<sup>7)</sup>

$$V_3(r, s, t) = \left[ -A e^{-a(r+s+t)} + \frac{C}{(rst)^3} \right] (1 + \cos \vartheta_1 \cdot \cos \vartheta_2 \cdot \cos \vartheta_3) \quad (\text{A9})$$

where

$$A = 1.336 \cdot 10^{-16} \text{ J}$$

$$C = 2.1005 \cdot 10^{-110} \text{ J m}^9$$

$$a = 1.936 \cdot 10^{10} \text{ m}^{-1}.$$

$r, s, t$  are distances between atoms, i. e. sides of a triangle whose angles are  $\vartheta_1, \vartheta_2$  and  $\vartheta_3$ . In a special case where  $r = s = t$  this potential is presented in Fig. 3.

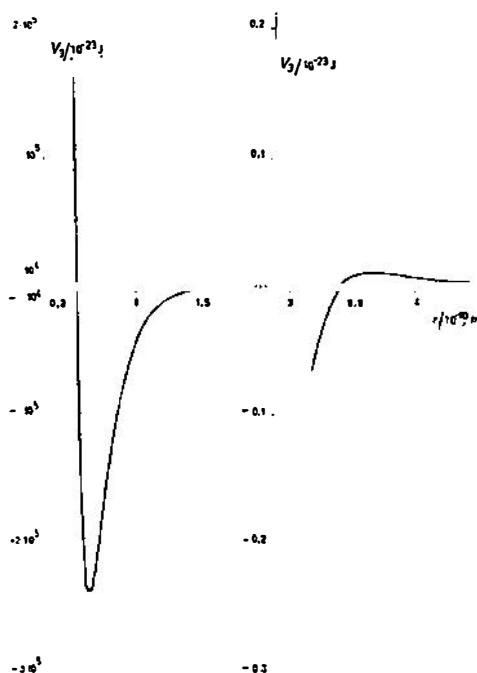


Fig. 3. Three-body potential among helium atoms.

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# RAZLIČITI POTENCIJALI I VIŠESTRUKKE KORELACIJE U TEKUĆEM $^4\text{He}$ U MODELU ATOMSKIH KUGLI

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Pokazano je da u granici malih gustoća u aproksimaciji čvrstih kugli dvočestična korelaciona funkcija koja minimizira energiju ima, za male međučestične udaljenosti, oblik  $u_2 \sim -\ln r^2 + \left(\frac{\alpha}{r}\right)^5$ . Nadalje je utvrđeno da u istom limesu Wu-Feenberg-Ljoljina dvočestična funkcija daje minimum energije za Maitland-Smithov potencijal i u odnosu na Lennard-Jones potencijal bolju za oko 9%. Također je utvrđeno da je utjecaj tripletnih korelacija u ovom modelu zanemariv te da tročestični potencijal daje doprinos veći od nule i manji je od 0.6% u odnosu na dvočestični.