ON THE PROBLEM OF SMALL NUMBER OF He^4 ATOMS

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Abstract. - Employing the iterative Monte Carlo calculation for the binding energy of the 4 atoms of He^4 we obtained the value $E = -0,8.10^{-23}$ J. The wave function used in the analysis includes the correlations of short-range $\exp(-(\alpha/r)^{\beta})$ and of long-range $\exp(-sr)$. A comparison of the results obtained for the trimer $(He^4)_3$ and for the molecule $(He^4)_4$ shows an increase in binding energy per atom, and consequently we can conclude that it is sufficient to observe approximately a hundred particles to define an infinite system in the Monte Carlo calculations.

1. Introduction

In a homogeneous system containing N particles ($N \to \infty$) with short-range forces acting between them, the behaviour of the system as a whole is essentially determined by the inter-correlation between neighbouring particles. In spite of this fact, today fundamental fluids theories somehow take into account the correlations between all the particles. At present there is no satisfactory theories of quantum fluids which considers the infinite system as a correlation in a group of neighbouring particles, and regards each group as an interacting system containing a finite number of particles. One attempt in that direction based on the generalized cell model of particles was made in a previous paper[1]. In general, the development of such a theory would obviously lead to the consideration of a group containing a small number of atoms. At the outset, when considering the problem of liquid helium, it was necessary to take into consideration the existence of helium dimers, the energy binding 3,4 ... 13 atoms, the structure of such systems etc. The problem of the existence of helium dimers and trimers has been dealt with in several papers [2-5].
Comparing the results for a finite number of particles presented in the above mentioned papers with results obtained using the model of semi-free gas of liquid helium[6-8], it can be noted that the results of the many-body

theory lead to valid conclusions about the existence of a stable molecule He^4 and the non-existence of a stable molecule He^3. Consequently, the energy per particle in the model of the semi-free gas has the following form[6-8]

$$\frac{E}{N} = \rho I_1 + \rho^2 I_2 + \dots \qquad \text{for } He^4$$

$$\frac{E}{N} = \rho^{2/3} I_{1F} + \rho I_{2F} + \dots \qquad \text{for } He^3.$$

As $I_1 < 0$ and $I_{1F} > 0$ in the limit $\rho \to 0$ the energy remains negative for He^4 and it becomes positive for He^3.

This paper examines the problem of 4 atoms He^4. After the derivation of the general formulas presented in Section 2, the results of the calculations and discussions are summarized in Section 3. The computation of energy demands a numerical solution of the nine-fold integral. The method we employed is actually an iterative Monte Carlo (MC) procedure and in literature it is known as "Vegas"[9].

2. Energy of four atoms He^4

The variational ansatz is defined by the expression

$$E = \frac{\langle\phi|H|\phi\rangle}{\langle\phi|\phi\rangle}, \qquad (1)$$

where ϕ is a symmetrical wave function, and H has the form

$$H = -\frac{\hbar^2}{2m}\sum_i \Delta_i + \frac{1}{2}\sum_{ij} V(r_{ij}) \qquad (2)$$

with $m = 6{,}624.10^{-27}$ kg.

The Lennard-Jones potential was chosen for the interaction potential:

$$V(r) = 4 \cdot \varepsilon \{(\sigma/r)^{12} - (\sigma/r)^6\}, \qquad (3)$$

where $\varepsilon = 14{,}1.10^{-23}$ J. and $\sigma = 2{,}556.10^{-10}$ m.

The Bijl-Jastrow function was taken as the variational function in the form suggested by K.Ljolje[10]

$$\phi(1,2,\dots n) = \prod_{i<j} \exp\{-(\alpha/r_{ij})^{\beta} - s r_{ij}\} ; \qquad (4)$$

α , β and s are the variational parameters. As the variational parameters α and

β were defined in the previous papers[11,12,5], only s is varied. The expected value of energy (1) with the wave function (4) can be written in the form:

$$E(s) = I_B/I_N \tag{5}$$

with

$$I_B = \int \psi H \psi d\tau = \int \psi^2 \{ -\frac{\hbar^2}{2m} \{ \sum_i \sum_j \sum_k (\alpha^\beta \beta . r_{ij}^{-\beta-1} - s)(\alpha^\beta . \beta . r_{ik}^{-\beta-1} - s) \frac{\vec{r}_{ij} . \vec{r}_{ik}}{r_{ij} . r_{ik}}$$

$$+ \sum_i \sum_j (\beta \alpha^\beta (1-\beta) r_{ij}^{-\beta-2} - 2sr_{ij}^{-1}) \} + 2.\varepsilon \sum_i \sum_j (\sigma / r_{ij})^6 ((\sigma / r_{ij})^6 - 1) \} d\tau \tag{5'}$$

$$\text{and} \quad I_N = \int \psi^2 \, d\tau = \int \exp\{ - \sum_i \sum_j ((\alpha / r_{ij})^\beta + s r_{ij}) \} d\tau \; . \tag{5''}$$

In order to restrict the computation to a finite part of the region and to eleminate the movement of the center of masses, the computation was carried out in Jacobi's coordinates[13]; when n = 4 Jacobi's coordinates are defined by the relations

$\xi_1 = x_1 - x_2$ $\qquad\qquad$ $\xi_3 = 1/3\ (x_1 + x_2 + x_3) - x_4$

$\xi_2 = 1/2\ (x_1 + x_2) - x_3$ $\qquad\qquad$ $\xi_4 = 1/4\ (x_1 + x_2 + x_3 + x_4)$.

Analogous relations are valid for η and ζ components. The inverse transformations are

$x_1 = 1/2\ \xi_1 + 1/3\ \xi_2 + 1/4\ \xi_3 + \xi_4$ $\qquad$ $x_3 = -\ 2/3\ \xi_2 + 1/4\ \xi_3 + \xi_4$

$x_2 = -1/2\ \xi_1 + 1/3\ \xi_2 + 1/4\ \xi_3 + \xi_4$ $\qquad$ $x_4 = -\ 3/4\ \xi_3 + \xi_4$.

The expressions for the y and z components are analogous. The Jacobian of the transformation is equal to 1. By integrating over the coordinates of the center of masses we obtain the volume V and the twelve-fold integrals are reduced to nine-fold integrals. The integrals are finally reduced to formulas which can be used in numerical computations transforming them into the interval $[0,1]$ for all the variables.

3. Results and Discussion

The computation of energy was performed using the above-mentioned iterative Monte Carlo procedure "Vegas"[9]. For particular values of parameter s the computation of the nominator took about 40 minutes, and for the denominator it took 7 minutes on the UNIVAC 1110. The results of the calculations are presented in the Table and Figure. For the value of parameter s of about $0{,}14.10^{10}\ m^{-1}$ the energy is at minimum and it is $E = -0{,}8.10^{-23}\ J$. The respective values of parameter s obtained for two particles in two-dimensional motion[5] $s = 0{,}075.10^{10}\ m^{-1}$ and in the three-dimensional case of 13 particles[10] $s = 0{,}17.10^{10}\ m^{-1}$ demonstrate that our results confirm the expected behaviour of the wave function in the four-particle system. The wave function binds the particles more strongly than in the case of two atoms and less strongly than in the system of 13 atoms.

s $10^{10}.m^{-1}$	$I_B.V^{-1}$ $10^{-38}.J$	St.dev. $10^{-38}J$	$I_N.V^{-1}$ 10^{15}	St.dev. 10^{15}	E $10^{-23}J$	St.dev. $10^{-23}J$
0,1	-0,2194	0,010	0,814	0,016	-0,2695	0,0176
0,12	-0,2319	0,0318	0,434	0,020	-0,534	0,097
0,14	-0,0215	0,0032	0,0266	0,0015	-0,806	0,165
0,16	-0,000356	0,000068	0,00799	0,000256	-0,0446	0,0099

Table. Values of the Vegas computation of integrals I_B, I_N and energy E for four atoms of He^4.

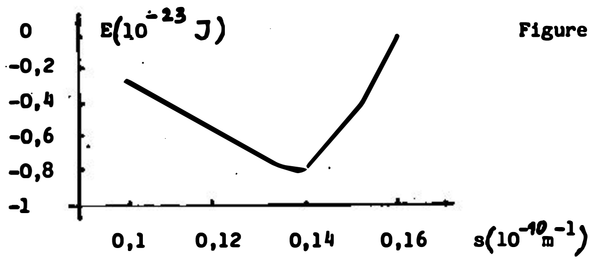

Figure. Energy of 4 atoms He^4 as the function of parameter s.

The binding energy of trimer He^4 is defined in paper[14] and is approximately $-0,138.10^{-23}$ J, i.e. $-0,046.10^{-23}$ J/atom. It is evident from the Table that the binding energy per one atom in a four-atom molecule of He^4 is not greater than $-0,16.10^{-23}$ J/atom. Consequently, the increase in binding energy per one atom is $-0,114.10^{-23}$ J./atom. Since the experimental binding energy per atom in liquid helium amounts to $-9,88.10^{-23}$ J/atom, we can conclude that 87 particles are sufficient to describe a real system. This result is only a qualitative orientation. All 87 particles cannot behave in the same way with regard to a single particale, since there are some first neighbour particles immediately surrounding it, then second neighbour particles etc. It should be emphasized that there is good agreement between the number we obtained and the Monte Carlo calculations of the infinite systems, and it is evident that it is sufficient to observe about a hundred particles in order to obtain results which approach experimental ones.

Another very interesting question is whether the atoms in a molecule of He^4, taking into account their strongly expressed wave properties, form fixed positions. This problem could be solved by computing the binding energy using the wave function that keeps the atoms fixed around firm positions in space. Otherwise it is difficult at present to connect the structure of the He^4 molecule with any known anorganic molecule in which atoms oscillate only slightly around the equilibrium positions. Bearing in mind the fact that the basic state of helium is liquid, the molecule $(He^4)_4$ can be considered a liquid structure in whieh the centers of the atoms are considerably mobile.

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