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A POTENTIAL ENERGY OF INTERACTION BETWEEN HELIUM ATOMS

I. O. Vakarchuk, V. V. Babin, A. A. Rovenchak
Ivan Franko National University of Lviv, Department of Theoretical Physics
12 Drahomanov Str., UA–79005, Lviv, Ukraine
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In the work the pair potential of interatomic interaction between helium atoms is established from the first principles without using fitting parameters. Previously obtained from Schrödinger equation connection between the potential Fourier image and the coefficient functions in the expansion of the many-boson system ground state wave function logarithm by the "degrees" of density fluctuations are used. RPA as the zero approximation and the approximation of "two sums over wave vector" as the first one are considered.

The results of this work lead to the value of the first sound velocity of 231 m/s while the experiment gives 237 m/s. The fit of our potential with Aziz model potential is quite good: the well depths are −10.58 K and −11.04 K respectively, the minimum positions being 3.34 Å and 2.99 Å.
Key words: liquid helium, interatomic potential, random-phase approximation, first sound.

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I. INTRODUCTION

When developing a theory of many particle systems from the first principles a key value in terms of the initial information is seen in the potential energy which predetermines the nature of the inter–particle interaction. It is generally assumed that it has a pair nature and is expressed through the sum of all the pair interactions between the particles. When speaking about the pair potential we virtually mean a certain effective two–particle interaction leading to an agreement between the theoretical results and the observed, yet fully neglected, many–particle interactions whose contribution into the thermodynamic functions of the system is known to be quite substantial in some cases [1,2].

There are several ways of establishing the potential energy. Firstly, we can accomplish this task via a direct quantum mechanics calculation. Secondly, we can accept a specified model form of the potential whose parameters are to be determined by an agreement between the calculated and observable values of physical quantities [3–5]. Another possibility arises when solving the inverse problem within the theory of particles scattering. Should the latter be coming into effect on the condensed matter bodies, the potential is recoverable by the experimental values of the so–called structure factor.

Within the classical approach [1,2] proceeding from the pair structure factor S_q of the N particles system it is easy to obtain a radial distribution function

$$F_2(r) = 1 + \frac{1}{N}\sum_{\mathbf{q}\neq 0}(S_q - 1)\exp(-i\mathbf{qr}).$$

We can further obtain the $\Phi(r)$ pair inter–particle potential in certain approximations by the known function $F_2(r)$ from Bogoliubov–Born–Green–Kirkwood–Ivon equation. Studies of this type were carried out for simple liquids such as argon or for liquid metals [2]. In the case of simple liquids a potential of the Lennard–Jones type was obtained, the so–called long–range interaction oscillating potentials having been received for liquid metals.

Reproducing the $\Phi(r)$ inter–particle interaction pair potential in ^{4}He from the experimental values of the S_q pair structure factor seems quite an interesting problem to solve. The classical scheme is understandably unfit for low temperatures owing to the fact that in this region ^{4}He is to be interpreted in terms of quantum mechanics.

II. INITIATING EXPRESSIONS

Our task consists in rediscovering $\Phi(r)$ from S_q calculated experimentally from the scattering of heat neutrons in the superfluid ^{4}He [8] within the framework of the quantum mechanics description. For this purpose one must possess a connection between the Fourier image of the pair interaction potential ν_q and S_q which is far more complex than in the classic case. The solution of this problem in the two sums approximation over the wave vector follows from the results obtained in [6,7] where a many–boson non–ideal system is considered at $T = 0$ K (i.e. in the ground state from the point of view of quantum mechanics). In [7] a sequence of equations was obtained for the coefficient functions $a_2, a_3, a_4, \ldots$ in the expansion of the many–boson system ground state wave function logarithm by the "degrees" of collective variables:

$$\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) = C\exp\left\{\sum_{n\geq 2}\frac{N^{1-n/2}}{n!}\sum_{\mathbf{k}_1\neq 0}\ldots\sum_{\mathbf{k}_n\neq 0}\delta(\mathbf{k}_1+\ldots+\mathbf{k}_n)a_n(\mathbf{k}_1,\ldots,\mathbf{k}_n)\rho_{\mathbf{k}_1}\ldots\rho_{\mathbf{k}_n}\right\},$$

$$\rho_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{-i\mathbf{k}\mathbf{r}_j}.$$

In the approximation of "two sums over the wave vector" we shall receive the following system of equations from Schrödinger equation (1–3):

$$\frac{N}{V}\frac{m\nu_k}{\hbar^2} + \mathbf{k}^2\, a_2(\mathbf{k}) - \mathbf{k}^2\, a_2^2(\mathbf{k}) - \frac{1}{2N}\sum_{\mathbf{q}\neq\mathbf{0}} \mathbf{q}^2\, a_4(\mathbf{q},-\mathbf{q},\mathbf{k},-\mathbf{k}) + \frac{1}{N}\sum_{\mathbf{q}\neq\mathbf{0}} \mathbf{q}(-\mathbf{k}-\mathbf{q})\, a_3(\mathbf{k},\mathbf{q},-\mathbf{k}-\mathbf{q}) = 0, \tag{1}$$

$$a_3(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3) = \frac{-2}{\mathbf{k}_1^2\,[1-2a_2(\mathbf{k}_1)] + \mathbf{k}_2^2\,[1-2a_2(\mathbf{k}_2)] + \mathbf{k}_3^2\,[1-2a_2(\mathbf{k}_3)]} \tag{2}$$
$$\times \Big\{\mathbf{k}_1\mathbf{k}_2\, a_2(\mathbf{k}_1)a_2(\mathbf{k}_2) + \mathbf{k}_1\mathbf{k}_3\, a_2(\mathbf{k}_1)a_2(\mathbf{k}_3) + \mathbf{k}_2\mathbf{k}_3\, a_2(\mathbf{k}_2)a_2(\mathbf{k}_3)\Big\},$$

$$a_4(\mathbf{k},-\mathbf{k},\mathbf{q},-\mathbf{q}) = \frac{1}{\mathbf{k}^2[1-2a_2(\mathbf{k})] + \mathbf{q}^2[1-2a_2(\mathbf{q})]}\Big\{(\mathbf{k}+\mathbf{q})^2 a_3^2(\mathbf{k}+\mathbf{q},-\mathbf{k},-\mathbf{q}) + (\mathbf{k}-\mathbf{q})^2 a_3^2(\mathbf{k}-\mathbf{q},-\mathbf{k},\mathbf{q}) \tag{3}$$
$$+\, 2[\mathbf{k}(\mathbf{k}+\mathbf{q})a_2(\mathbf{k}) + \mathbf{q}(\mathbf{q}+\mathbf{k})a_2(\mathbf{q})]\, a_3(\mathbf{k}+\mathbf{q},-\mathbf{k},-\mathbf{q}) + 2[\mathbf{k}(\mathbf{k}-\mathbf{q})a_2(\mathbf{k}) + \mathbf{q}(\mathbf{q}-\mathbf{k})a_2(\mathbf{q})]\, a_3(\mathbf{k}-\mathbf{q},-\mathbf{k},+\mathbf{q})\Big\}.$$

Here we shall skip over the expressions obtained for the s-particle density matrices $F_s(\mathbf{r}_1,\ldots,\mathbf{r}_s)$ through the functions a_2, a_3, a_4 from [7]. Hence, taking into account the simple connection of the pair distribution function and the pair structure factor of the system this implies a correlation in the approximation of "the two sums over the wave vector" between a_2, a_3, a_4 and S_q at the absolute zero temperature:

$$a_2(\mathbf{q}) = \frac{1}{2}\left(1 - \frac{1}{S_q}\right) - \frac{1}{2}\Sigma(\mathbf{q}), \tag{4}$$

where $\Sigma(\mathbf{q})$ is a complex functional of a_2:

$$\Sigma(\mathbf{q}) = \frac{2}{N}\sum_{\substack{\mathbf{k}_1\neq 0\ \mathbf{k}_2\neq 0\\ \mathbf{k}_1+\mathbf{k}_2+\mathbf{q}=0}} \frac{1}{[1-2a_2(\mathbf{k}_1)]\,[1-2a_2(\mathbf{k}_2)]}\Big\{a_2(\mathbf{k}_1)a_2(\mathbf{k}_2) + a_3(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q})\,[1+a_3(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q})]\Big\} \tag{5}$$
$$+\, \frac{1}{N}\sum_{\mathbf{k}\neq 0}\frac{a_4(\mathbf{k},-\mathbf{k},\mathbf{q},-\mathbf{q})}{[1-2a_2(\mathbf{k})]}.$$

In correlation (4) it will suffice to calculate the value of $\Sigma(\mathbf{q})$ on the functions $a_2(\mathbf{q})$ in the random phase approximation

$$a_2(\mathbf{q}) = \frac{1}{2}\left(1 - \frac{1}{S_q}\right). \tag{6}$$

Next, we shall determine the Fourier image ν_q of the potential in the accepted approximation from (1). For a_3, a_4 it is enough to be confined by the RPA which means that we shall embed the a_2 value determined from (6) into the right–hand side of (2) and (3). We shall execute the transition into $\Phi(\mathbf{r})$ in a usual way

$$\Phi(r) = \frac{1}{V}\sum_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}}\nu_q. \tag{7}$$

III. RESULTS AND THEIR DISCUSSION

For carrying out numerical calculations we made use of the experimental values of the superfluid ^{4}He structure factor from [8] which correspond to the density value of $\rho = 0.02185$ Å^{-3} and to the temperature $T = 1$ K. As the initial expressions contain S_q at $T = 0$ K we converted these values into those at $T = 0$ K falling back on correlation [9]

$$S_q = S_q(T) \tanh \frac{E_q}{2T},$$

$$E_q = \frac{\hbar^2 q^2}{2mS_q},$$

$$S_q = S_q\big|_{T=0},$$

which were treated as equations for S_q at the given $S_q(T)$. A plot of the smooth structure factor from [8] as well as S_q is given in Fig. 1 that corresponds to Table 1.

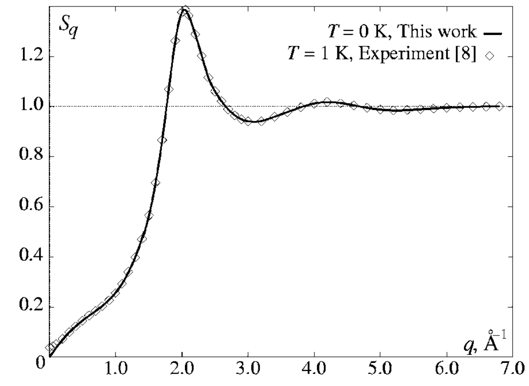

Fig. 1. The ^{4}He structure factor.

	$r_{\min}$, Å	$\Phi(r_{\min})$, K	$\Phi(0)$, K
RPA	3.31	-17.08	$\simeq 242$
1st approximation	3.34	-10.58	$\simeq 230$
Aziz model potential [5]	2.99	-11.04	$\simeq 2 \cdot 10^6$
Lennard–Jones potential [10]	2.556	-10.22	∞

Table 1. Comparison of the results.

Making use of S_q received in this fashion we carried out a calculus of ν_q and $\Phi(r)$ in the random phase approximation and the subsequent approximation of "two sums over the wave vector". The random phase approximation implies that it is necessary to discard all the terms which contain the sums over the wave vector from (1) and to take a_2 from (6), i. e.

$$\nu_q = \frac{\hbar^2 q^2}{2m} \frac{1}{2\rho} \left(\frac{1}{S_q^2} - 1 \right). \tag{8}$$

The results of the calculations are adduced in Tables 2–4 and Figs. 2–4.

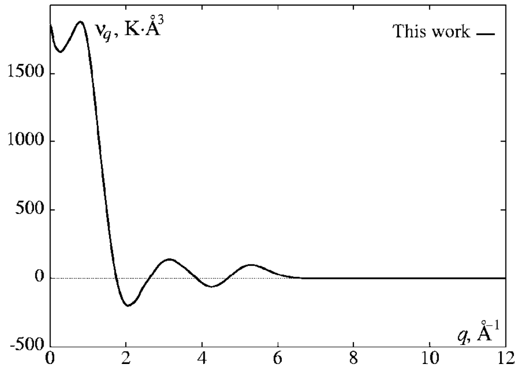

Fig. 2. The Fourier image of the potential of interatomic interaction in ^{4}He .

It is interesting to establish the first sound velocity c from the obtained ν_0 in superfluid ^{4}He making use of Bogoliubov equation:

$$c = \sqrt{\frac{\rho \nu_0}{m}}. \tag{9}$$

We shall obtain the value of c at 291 m/s whereas its experimental value c^{exp} equals 237 m/s. The first correction to (9) (see [6]) leads to $c = 231$ m/s which is a very satisfactory result.

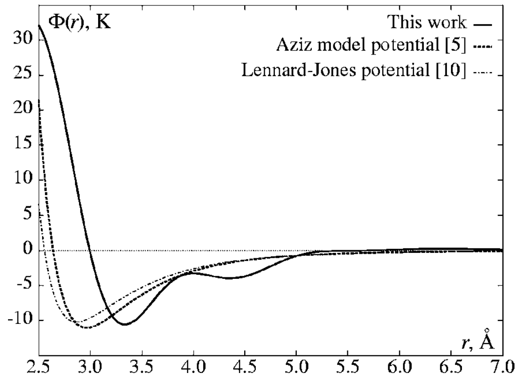

Fig. 3. The potential of interatomic interaction, comparison with model potentials.

Fig. 3 shows Aziz model potential for the sake of comparison [5] together with Lennard–Jones potential [10]. The potential in two approximations is presented in Fig. 4. Due to the restriction of experiment only the finite maximum value of the wave vector q is available for carrying out the calculation in (7). Therefore, the numerical results for $\Phi(r)$ at small distances should not be considered as quite correct just as the "waves" at $r \simeq 2$ Å.

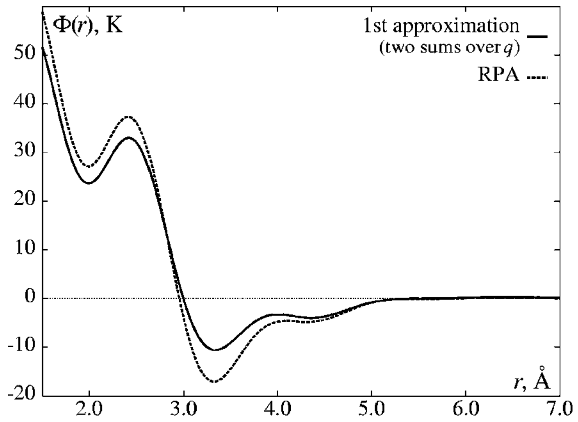

Fig. 4. The potential of interatomic interaction, comparison of approximations.

Partly they are the consequence of the experimental restriction mentioned above and partly they should be eliminated by taking into account many–particle effects. On the other hand, one can consider those $\Phi(r)$ values as non–significant since their contribution into the statistical operator is negligible in the temperature region where ^{4}He stays liquid.

As can be seen from Fig. 4 and Table 3 the approximation of the two sums over the wave vector tangibly improves the value for the well depth of the potential leaving almost intact the position of the potential minimum (the distances between the atoms being equally balanced) in comparison with the random phase approximation. Otherwise stated, the influence of three– and four–particle correlations proves to be considerable.

The findings obtained in this paper are to be used for developing a theory from the first principles.

APPENDIX

q, Å^{-1}	S_q	q, Å^{-1}	S_q	q, Å^{-1}	S_q	q, Å^{-1}	S_q
0.00	0.000	1.65	0.775	3.30	0.949	4.95	0.989
0.05	0.017	1.70	0.865	3.35	0.954	5.00	0.988
0.10	0.033	1.75	0.965	3.40	0.959	5.05	0.987
0.15	0.053	1.80	1.069	3.45	0.964	5.10	0.986
0.20	0.069	1.85	1.172	3.50	0.969	5.15	0.985
0.25	0.084	1.90	1.263	3.55	0.973	5.20	0.985
0.30	0.098	1.95	1.334	3.60	0.978	5.25	0.985
0.35	0.111	2.00	1.377	3.65	0.983	5.30	0.985
0.40	0.123	2.05	1.387	3.70	0.988	5.35	0.986
0.45	0.134	2.10	1.365	3.75	0.992	5.40	0.986
0.50	0.145	2.15	1.330	3.80	0.997	5.45	0.987
0.55	0.155	2.20	1.290	3.85	1.001	5.50	0.988
0.60	0.165	2.25	1.248	3.90	1.005	5.55	0.989
0.65	0.175	2.30	1.203	3.95	1.009	5.60	0.990
0.70	0.184	2.35	1.157	4.00	1.012	5.65	0.991
0.75	0.194	2.40	1.116	4.05	1.014	5.70	0.992
0.80	0.204	2.45	1.085	4.10	1.016	5.75	0.993
0.85	0.215	2.50	1.061	4.15	1.018	5.80	0.994
0.90	0.227	2.55	1.040	4.20	1.018	5.85	0.995
0.95	0.241	2.60	1.021	4.25	1.018	5.90	0.995
1.00	0.256	2.65	1.004	4.30	1.017	5.95	0.996
1.05	0.273	2.70	0.989	4.35	1.016	6.00	0.997
1.10	0.293	2.75	0.976	4.40	1.014	6.05	0.997
1.15	0.315	2.80	0.965	4.45	1.012	6.10	0.998
1.20	0.340	2.85	0.956	4.50	1.010	6.15	0.998
1.25	0.368	2.90	0.949	4.55	1.007	6.20	0.999
1.30	0.399	2.95	0.944	4.60	1.005	6.25	0.999
1.35	0.433	3.00	0.941	4.65	1.002	6.30	0.999
1.40	0.472	3.05	0.939	4.70	1.000	6.35	1.000
1.45	0.515	3.10	0.939	4.75	0.997	6.40	1.000
1.50	0.566	3.15	0.940	4.80	0.995	6.45	1.000
1.55	0.626	3.20	0.942	4.85	0.993	6.50	1.000
1.60	0.695	3.25	0.945	4.90	0.991	6.55	1.000

Table 2. Liquid helium-4 structure factor at $T = 0$ K.

q, Å^{-1}	ν_q, K·Å^3	q, Å^{-1}	ν_q, K·Å^3	q, Å^{-1}	ν_q, K·Å^3	q, Å^{-1}	ν_q, K·Å^3
0.00	1854.642	3.30	127.463	6.60	1.384	9.90	0.267
0.10	1718.064	3.40	107.952	6.70	0.142	10.00	0.322
0.20	1668.719	3.50	87.575	6.80	−0.649	10.10	0.365
0.30	1658.420	3.60	66.019	6.90	−1.121	10.20	0.392
0.40	1696.887	3.70	41.253	7.00	−1.360	10.30	0.402
0.50	1741.339	3.80	14.865	7.10	−1.436	10.40	0.398
0.60	1797.841	3.90	−11.037	7.20	−1.360	10.50	0.381
0.70	1855.320	4.00	−33.892	7.30	−1.178	10.60	0.355
0.80	1878.750	4.10	−51.770	7.40	−0.920	10.70	0.320
0.90	1841.081	4.20	−61.046	7.50	−0.612	10.80	0.281
1.00	1711.954	4.30	−60.682	7.60	−0.282	10.90	0.240
1.10	1510.052	4.40	−52.211	7.70	0.041	11.00	0.200
1.20	1254.183	4.50	−37.724	7.80	0.333	11.10	0.161
1.30	985.829	4.60	−18.491	7.90	0.575	11.20	0.127
1.40	732.031	4.70	5.239	8.00	0.754	11.30	0.097
1.50	492.149	4.80	30.105	8.10	0.869	11.40	0.072
1.60	261.975	4.90	53.630	8.20	0.908	11.50	0.051
1.70	74.959	5.00	73.707	8.30	0.884	11.60	0.035
1.80	−62.007	5.10	89.292	8.40	0.807	11.70	0.023
1.90	−148.885	5.20	98.210	8.50	0.692	11.80	0.014
2.00	−193.077	5.30	100.844	8.60	0.554	11.90	0.008
2.10	−198.860	5.40	97.782	8.70	0.406	12.00	0.004
2.20	−178.040	5.50	90.167	8.80	0.263	12.10	0.001
2.30	−141.568	5.60	79.563	8.90	0.139	12.20	−0.000
2.40	−85.980	5.70	67.075	9.00	0.040	12.30	−0.001
2.50	−42.129	5.80	54.289	9.10	−0.032	12.40	−0.002
2.60	−1.734	5.90	42.231	9.20	−0.067	12.50	−0.002
2.70	39.482	6.00	31.578	9.30	−0.070	12.60	−0.001
2.80	78.124	6.10	22.495	9.40	−0.046	12.70	−0.001
2.90	110.073	6.20	15.420	9.50	0.000	12.80	−0.001
3.00	130.602	6.30	10.042	9.60	0.061	12.90	−0.001
3.10	141.836	6.40	6.110	9.70	0.131	13.00	−0.000
3.20	140.580	6.50	3.337	9.80	0.202	13.10	−0.000

Table 3. The Fourier image of the interatomic potential in ^{4}He.

r, Å	$\Phi(r)$, K	r, Å	$\Phi(r)$, K	r, Å	$\Phi(r)$, K	r, Å	$\Phi(r)$, K
0.00	(229.852)	3.80	−4.250	7.70	0.041	11.50	−0.039
0.10	(222.056)	3.90	−3.487	7.80	0.050	11.60	−0.038
0.20	200.262	4.00	−3.261	7.90	0.067	11.70	−0.036
0.30	168.745	4.10	−3.406	8.00	0.092	11.80	−0.033
0.40	133.153	4.20	−3.695	8.10	0.120	11.90	−0.030
0.50	99.024	4.30	−3.917	8.20	0.150	12.00	−0.028
0.60	70.679	4.40	−3.931	8.30	0.178	12.10	−0.025
0.70	50.694	4.50	−3.685	8.40	0.199	12.20	−0.022
0.80	39.840	4.60	−3.206	8.50	0.213	12.30	−0.018
0.90	37.253	4.70	−2.579	8.60	0.216	12.40	−0.014
1.00	40.735	4.80	−1.908	8.70	0.209	12.50	−0.010
1.10	47.228	4.90	−1.287	8.80	0.192	12.60	−0.005
1.20	53.506	5.00	−0.783	8.90	0.167	12.70	−0.000
1.30	56.975	5.10	−0.422	9.00	0.137	12.80	0.005
1.40	56.302	5.20	−0.198	9.10	0.104	12.90	0.010
1.50	51.624	5.30	−0.082	9.20	0.071	13.00	0.014
1.60	44.279	5.40	−0.034	9.30	0.041	13.10	0.018
1.70	36.209	5.50	−0.017	9.40	0.016	13.20	0.021
1.80	29.316	5.60	−0.004	9.50	−0.003	13.30	0.023
1.90	24.954	5.70	0.020	9.60	−0.014	13.40	0.025
2.00	23.656	5.80	0.058	9.70	−0.020	13.50	0.025
2.10	25.074	5.90	0.107	9.80	−0.019	13.60	0.025
2.20	28.115	6.00	0.159	9.90	−0.015	13.70	0.024
2.30	31.250	6.10	0.204	10.00	−0.009	13.80	0.023
2.40	32.953	6.20	0.237	10.10	−0.003	13.90	0.022
2.50	32.134	6.30	0.256	10.20	0.003	14.00	0.020
2.60	28.437	6.40	0.262	10.30	0.007	14.10	0.018
2.70	22.283	6.50	0.256	10.40	0.008	14.20	0.016
2.80	14.660	6.60	0.243	10.50	0.006	14.30	0.013
2.90	6.784	6.70	0.224	10.60	0.002	14.40	0.010
3.00	−0.238	6.80	0.203	10.70	−0.005	14.50	0.007
3.10	−5.631	6.90	0.180	10.80	−0.012	14.60	0.003
3.20	−9.036	7.00	0.156	10.90	−0.019	14.70	0.000
3.30	−10.486	7.10	0.131	11.00	−0.026	14.80	−0.003
3.40	−10.320	7.20	0.107	11.10	−0.032	14.90	−0.005
3.50	−9.064	7.30	0.084	11.20	−0.036	15.00	−0.007
3.60	−7.308	7.40	0.064	11.30	−0.039	15.10	−0.007
3.70	−5.580	7.50	0.049	11.40	−0.040	15.20	−0.007

Table 4. The potential of the interatomic interaction in ^{4}He.

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ПОТЕНЦІЯЛЬНА ЕНЕРҐІЯ ВЗАЄМОДІЇ МІЖ АТОМАМИ ГЕЛІЮ

І. О. Вакарчук, В. В. Бабін, А. А. Ровенчак

Львівський національний університет імені Івана Франка

Кафедра теоретичної фізики

вул. Драгоманова, 12, 79005, Львів, Україна

У роботі з перших принципів та без використання допоміжних параметрів отримано парний потенціял міжатомної взаємодії для гелію. При цьому застосовано знайдені раніше з рівняння Шредингера співвідношення, які пов'язують Фур'є–зображення потенціялу з коефіцієнтними функціями в розкладі лоґарифма хвильової функції основного стану багатобозонної системи за степенями флюктуацій густини. Розглянуті RPA-наближення як нульова та наближення "двох сум за хвильовим вектором" як перша апроксимація.

З результатів роботи випливає значення швидкости першого звуку 231 м/с, тоді як експеримент дає 237 м/с. Узгодження нашого потенціялу з модельним потенціялом Азіза є цілком задовільним: глибини потенціяльних ям становлять відповідно -10.58 К та -11.04 К, точки мінімуму — 3.34 Å та 2.99 Å.