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SURFACE PROPERTIES OF LIQUID ^{3}He AT ZERO PRESSURE

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Abstract: Surface properties of quantum liquids have constituted a field for numerous interesting investigations, both experimental and theoretical. In this paper we study contribution of various nearest neighbours in simple cubic arrangement of the liquid helium toward the surface tension ($\boldsymbol{\sigma}$) of liquid ^{3}He. To this effect we use standard inter-atomic potential (Lennard Jones potential). We note that the major part of the contribution comes from its first four nearest neighbours. The agreement between our theoretical results with experimental values is satisfactory.

Keywords: ^{3}He; simple cubic; nearest neighbour; surface tension.

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1. Introduction:

Liquid ^{3}He is an exceptional system: at sufficiently low temperatures its normal phase is the prototype of Landau Fermi liquid [1], while the superfluid phases appearing at even lower temperatures presents example of anisotropic BCS-type superfluids [1-3]. Therefore liquid ^{3}He has been investigated systematically and in considerable detail at temperature T both below the critical temperature T_C in the superfluid state ($T < T_C = 0.0026$ K) and in Fermi liquid regime ($T_C < T \leq 0.16$ K) [3-5].

Liquid ^{3}He system has given an opportunity to examine the quantum effects at macroscopic level; one such effect being the thermodynamic properties (like entropy, thermal expansion coefficients, specific heat, surface tension etc.) and their dependence on molar volume V and pressure P are being studied and discussed by various authors [5,6]. In this paper we will discuss one of the utmost important thermodynamic property surface tension at P=0 bar.

2. Our approach:

Surface tension is a property of the surface of a liquid and is defined as the excess energy available per unit area. To calculate the surface tension (σ), each particle in the system is considered to be a particle trapped in spherical cavity formed by its nearest neighbour atoms in simple cubic (SC) arrangement. Surface tension (σ) of the liquid has been obtained from the difference of the potential energy of ^{3}He atom at the liquid surface and that well below the surface. To this effect we use standard inter-atomic potential (Lennard Jones potential). We note that the major part of the potential energy contribution comes from nearest neighbours [7- 9].

The helium atoms interact through the Lennard-Jones potential given by [2-4]

$$\mathbf{V}(\mathbf{r_{ij}}) = \mathbf{4}\boldsymbol{\epsilon}\left[\left(\frac{\mathbf{a}}{(\mathbf{r_{ij}})}\right)^{\mathbf{12}} - \left(\frac{\mathbf{a}}{(\mathbf{r_{ij}})}\right)^{\mathbf{6}}\right] \tag{1}$$

where $\boldsymbol{\epsilon}$=10.22 K and a=2.556 A^o. These two parameters depend on polarizability and average dipole moment of an atom as well as on the core overlap.

The total potential V is given by

$$\mathbf{V} = \frac{\mathbf{1}}{\mathbf{2}}\sum\nolimits_{\mathbf{ij}} \mathbf{V}(\mathbf{r_{ij}}) \tag{2}$$

The factor 1/2 takes care of repetition in i and j.

If n_{ij} is the number of particle at a distance P_{ij} d, the contribution of these atoms to the potential of i^{th} particle is

$$\mathbf{V(P_{ij}) = 2\epsilon\left[\left(\frac{\sigma}{d}\right)^{12}\frac{n_{ij}}{P_{ij}^{12}} - \left(\frac{\sigma}{d}\right)^{6}\frac{n_{ij}}{P_{ij}^{6}}\right]} \tag{3}$$

The total potential energy per particle can be estimated by considering the contribution from the atoms situated at all possible $P_{ij.}$

The above equation gives the potential energy when the atom is well within the liquid. However potential energy per particle reduces on the surface because for every P_{ij} there is a lack of contribution from $(n_{ij} - n_p)/2$ atoms where n_p is the number of atom at P_{ij}d at the plane surface

$$\mathbf{V_s(P_{ij}) = \frac{(n_{ij}+n_p)}{2}\,V(P_{ij})} \tag{4}$$

The total potential energy on the surface is obtained by considering the contribution of all P_{ij}.

Calculation of surface tension: In an atom liquid surface is always at higher potential in comparison to its counterpart well within the liquid the excess potential energy at an atomic location on the liquid surface due to the atoms for particular P_{ij} is

$$\mathbf{V_e(P_{ij}) = -\frac{n_{ij}-n_p}{2}V(P_{ij})} \tag{5}$$

and σ is the consequence of excess energy.

The total excess energy per atom V_e can be obtained taking into the contribution from all possible P_{ij}. V_e per unit area gives σ and can be estimated calculating the surface area available on an atom on the surface [8,9].

3. Results and discussion:

The parameters needed for the calculation of potential energy such as P_{ij}, n_{ij}, n_p for SC arrangement is given in table 1. In this table we have listed the possible values of P_{ij} for a given number of atoms located in the same horizontal plane (n_p) as well as the number of atoms in the 1^{st} (n_{p1}); 2^{nd} (n_{p2}); 3^{rd} (n_{p3}) horizontal plane upto the 10^{th} neighbourhood.

Table 1: Values of P_{ij} and corresponding numbers of atoms [8].

Number of Atoms					
	Total	**0^{th} Plane**	**1^{st} Plane**	**2^{nd} Plane**	**3^{rd} Plane**
P_{ij}	**n_{ij}**	**n_p**	**n_{p1}**	**n_{p2}**	**n_{p3}**
1.000	6	4	2	0	0
1.414	12	4	8	0	0
1.732	8	0	8	0	0
2.000	6	4	0	2	0
2.236	24	8	8	8	0
2.449	24	0	16	8	0
2.824	12	4	0	8	0
3.000	30	4	8	16	2
3.162	24	8	8	0	8
3.317	24	0	16	0	8

Table 2 lists the potential energy per particle (V_p) for normal-liquid ^{3}He at pressure P=0 bar for SC arrangement and its contribution from each neighbour. In table 3 the potential energy per particle on the surface (V_s) by each nearest neighbour are listed. Total excess energy per particle (V_e) for normal-liquid ^{3}He and the contribution from its nearest neighbour in SC arrangement are listed in table 4. Surface tension is estimated from the excess energy value.

Table 2: Potential energy per particle for normal-liquid ^{3}He at pressure P=0 bar for SC arrangement.

T (K)	**V_{p1}**	**V_{p2}**	**V_{p3}**	**V_{p4}**	**V_{p5}**	**V_{p6}**	**V_{p7}**	**V_{p8}**	**V_{p9}**	**V_{p10}**	**V_p**
0.0	-8.46	-2.27	-0.45	-0.14	-0.29	-0.17	-0.04	-0.06	-0.04	-0.03	-11.94
0.5	-8.58	-2.30	-0.46	-0.14	-0.30	-0.17	-0.04	-0.06	-0.04	-0.03	-12.12
1.0	-8.46	-2.27	-0.45	-0.14	-0.29	-0.17	-0.04	-0.06	-0.04	-0.03	-11.94
1.4	-8.23	-2.20	-0.44	-0.14	-0.28	-0.16	-0.03	-0.06	-0.04	-0.03	-11.61

1.8	-7.89	-2.10	-0.42	-0.13	-0.27	-0.16	-0.03	-0.06	-0.03	-0.03	-11.12
2	-7.67	-2.04	-0.41	-0.13	-0.26	-0.15	-0.03	-0.06	-0.03	-0.02	-10.81
2.4	-7.06	-1.87	-0.37	-0.12	-0.24	-0.14	-0.03	-0.05	-0.03	-0.02	-9.93
2.8	-6.08	-1.59	-0.32	-0.10	-0.21	-0.12	-0.03	-0.04	-0.03	-0.02	-8.52
3	-5.38	-1.40	-0.28	-0.09	-0.18	-0.10	-0.02	-0.04	-0.02	-0.02	-7.54
3.2	-4.59	-1.19	-0.24	-0.07	-0.15	-0.09	-0.02	-0.03	-0.02	-0.01	-6.42

Table 3: Potential energy per particle on the surface for normal-liquid ^{3}He at pressure P=0 bar for SC arrangement

T (K)	V_{S1}	V_{S2}	V_{S3}	V_{S4}	V_{S5}	V_{S6}	V_{S7}	V_{S8}	V_{S9}	V_{S10}	V_S
0.0	-12.69	-3.40	-0.68	-0.21	-0.58	-0.25	-0.05	-0.16	-0.07	-0.05	-18.16
0.5	-12.87	-3.45	-0.69	-0.22	-0.59	-0.26	-0.05	-0.16	-0.07	-0.06	-18.42
1.0	-12.69	-3.40	-0.68	-0.21	-0.58	-0.25	-0.05	-0.16	-0.07	-0.05	-18.16
1.4	-12.34	-3.30	-0.66	-0.21	-0.57	-0.25	-0.05	-0.15	-0.07	-0.05	-17.64
1.8	-11.83	-3.15	-0.63	-0.20	-0.54	-0.24	-0.05	-0.15	-0.07	-0.05	-16.90
2	-11.51	-3.06	-0.61	-0.19	-0.53	-0.23	-0.05	-0.14	-0.07	-0.05	-16.43
2.4	-10.59	-2.80	-0.56	-0.18	-0.48	-0.21	-0.04	-0.13	-0.06	-0.05	-15.10
2.8	-9.11	-2.39	-0.47	-0.15	-0.41	-0.18	-0.04	-0.11	-0.05	-0.04	-12.96
3	-8.07	-2.11	-0.42	-0.13	-0.36	-0.16	-0.03	-0.10	-0.05	-0.03	-11.46
3.2	-6.89	-1.78	-0.35	-0.11	-0.31	-0.13	-0.03	-0.08	-0.04	-0.03	-9.75

Table 4: Excess surface energy per particle for normal-liquid ^{3}He at pressure P=0 bar for SC arrangement.

T (K)	V_{e1}	V_{e2}	V_{e3}	V_{e4}	V_{e5}	V_{e6}	V_{e7}	V_{e8}	V_{e9}	V_{e10}	V_e
0.0	4.23	1.13	0.23	0.07	0.29	0.08	0.02	0.09	0.04	0.03	6.21
0.5	4.29	1.15	0.23	0.07	0.30	0.09	0.02	0.10	0.04	0.03	6.30
1.0	4.23	1.13	0.23	0.07	0.29	0.08	0.02	0.09	0.04	0.03	6.21
1.4	4.11	1.10	0.22	0.07	0.28	0.08	0.02	0.09	0.04	0.03	6.04
1.8	3.94	1.05	0.21	0.07	0.27	0.08	0.02	0.09	0.03	0.03	5.78
2	3.84	1.02	0.20	0.06	0.26	0.08	0.02	0.08	0.03	0.02	5.62
2.4	3.53	0.93	0.19	0.06	0.24	0.07	0.01	0.08	0.03	0.02	5.16
2.8	3.04	0.80	0.16	0.05	0.21	0.06	0.01	0.07	0.03	0.02	4.43
3	2.69	0.70	0.14	0.04	0.18	0.05	0.01	0.06	0.02	0.02	3.92
3.2	2.30	0.59	0.12	0.04	0.15	0.04	0.01	0.05	0.02	0.01	3.33

The percentage contributions by various neighbours towards three different energies are listed in table 5. The energy contribution from 1st neighbour is approximately 70%, while from 2nd neighbour it is ~19%, the 3rd neighbour contributes around 4%, ~1.2% is contributed by 4th neighbour while the 10th neighbour contributes only ~0.4%. The energy contribution by each neighbour decreases with increase in neighbour distance (P_{ij}). The significant contribution can be seen upto 6th neighbour (i.e. upto inter atomic distance of 2.449 A^o). The percentage contribution of various nearest neighbours towards V_p, V_s and V_e are plotted in figure 1.

Table 5: Percentage of nearest neighbour contribution towards potential energy per particle, Potential energy per particle on the surface and Excess surface energy per particle for normal-liquid ^{3}He at pressure P=0 bar for SC arrangement.

n	V_p	V_S	V_e
1	70.8	69.9	68.1
2	19.0	18.7	18.2
3	3.8	3.7	3.6
4	1.2	1.2	1.1
5	2.4	3.2	4.7
6	1.4	1.4	1.4
7	0.3	0.3	0.3
8	0.5	0.9	1.5
9	0.3	0.4	0.6
10	0.2	0.3	0.4

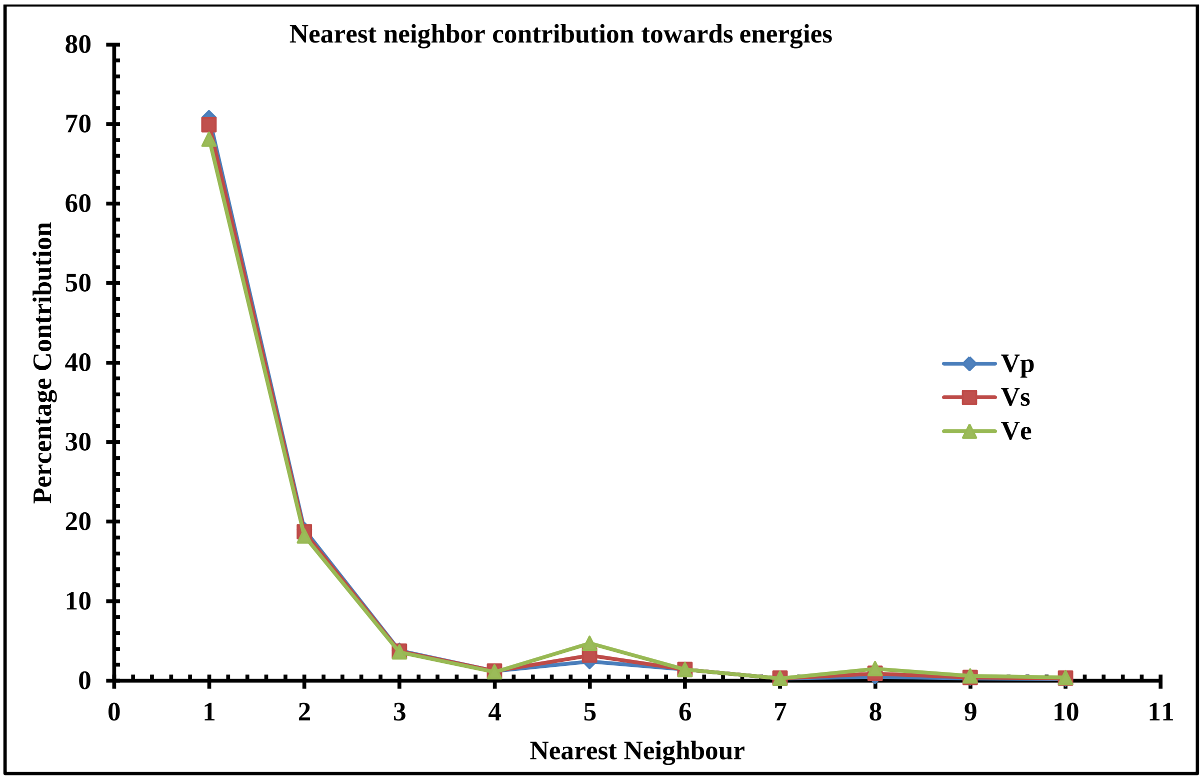

Figure 1: Percentage of nearest neighbour contribution towards Potential energy per particle (V_P), Potential energy per particle on the surface (V_s) and Excess surface energy per particle (V_e) for normal-liquid ^{3}He at pressure P=0 bar SC arrangement

The surface tension variation with temperatures for normal-liquid ^{3}He at pressure P=0 bar is shown in figure 2. In the temperature region $T \leq 1.5$ K our calculated values for σ are matching with the experimental data of Zinoveva [10], while for $T > 1.5$ K the calculated values are higher than the compared experimental data by more than 25%.

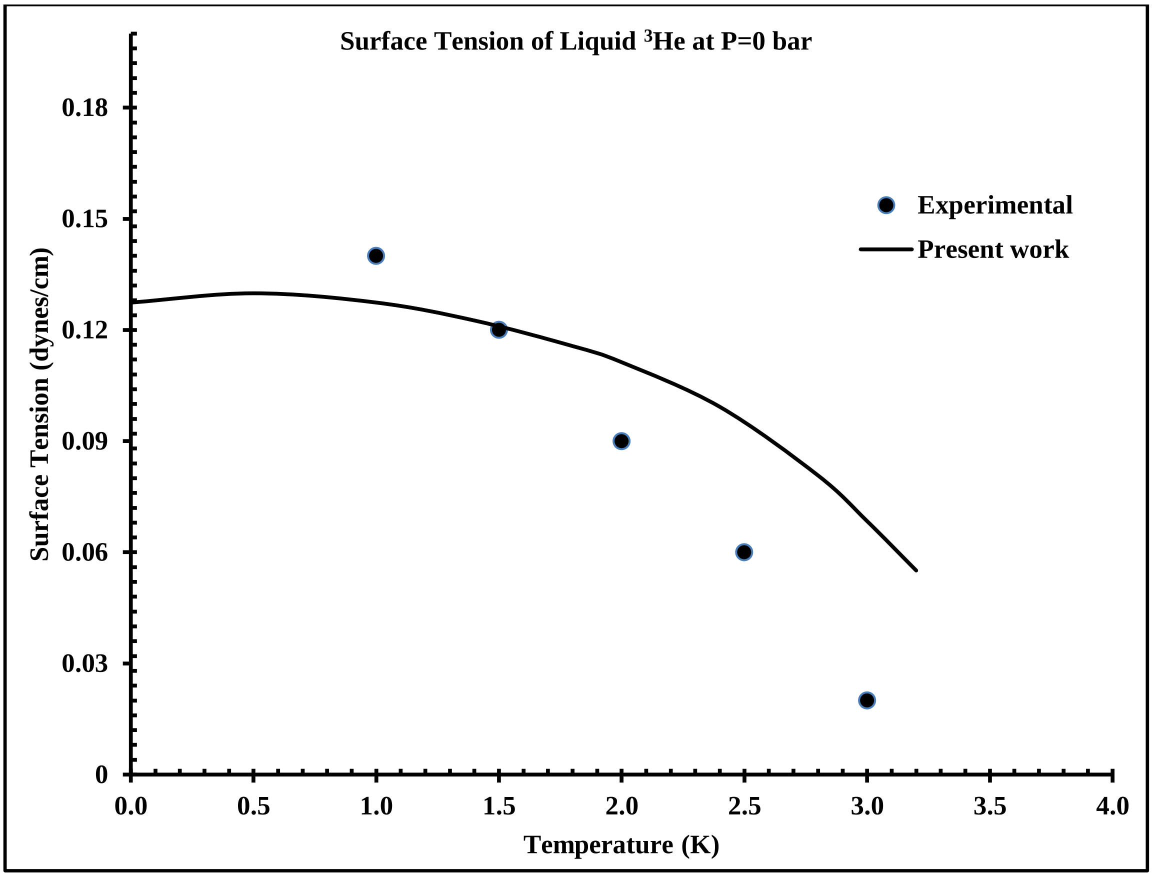

Figure 2: Variation of surface tension of for normal-liquid ^{3}He at pressure P=0 bar with temperatures.

4. Conclusion:

Our calculation is for static structure. We, therefore, attributed the difference between the calculated and the experimental value to the smaller density of helium atoms near the surface, to the thermal fluctuations in density and also to the difference in zero point motions of atoms near the surface and in the bulk. Our σ values also do not include the effects of parameters such as change of atomic layer separation near the surface of the liquid.

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