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## Evaluation of pressure dependent chemical potential of helium atom in liquid $^3\text{He}$

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Received 15 October 1999; revised 24 May 2000; accepted 7 June 2000

Using Mishra and Tripathy model Hamiltonian (*J. Low Temp. Phys.*, JLT P 75, 79 (1989)), the pressure dependent chemical potential of Helium atom has been evaluated in liquid  $^3\text{He}$ . The result show that chemical potential of helium atom in liquid increases with pressure, which are in satisfactory agreement with the experimental data at least for higher pressure. For low pressure, as per experimental observation negative value of chemical potential is not obtained. This is because Mishra and Tripathy model Hamiltonian is based on repulsive nature of potential. Taking more realistic potential having both repulsive and attractive part, the negative behaviour of the chemical potential of  $^3\text{He}$  atom in liquid  $^3\text{He}$  is observed.

### Introduction

Liquid  $^3\text{He}$  (which is known to be a Fermi liquid) behaves as a quantum system in the neighbourhood of extremely low temperatures. In this system, the interparticle potential consists of strong hard core repulsion plus a weak Van der Waal's attraction. There are two types of collective modes<sup>1</sup> in this system known as first sound mode and zero-sound mode. Both of these sound modes are due to the density fluctuation or due to distortion in the Fermi surfaces. The velocities of these sound modes have been measured experimentally<sup>2,3</sup> and are found to be equal; to 187 m/s and 194 m/s. These collective modes have been confirmed through inelastic neutron scattering measurements<sup>4-9</sup> both as a function of momentum transfer  $k$  and also for different pressures. Chemical potentials for liquid  $^4\text{He}$  and liquid  $^3\text{He}$  have been studied experimentally<sup>10,11</sup>. It has been observed that chemical potential of  $^3\text{He}$  and  $^4\text{He}$  increases with increase of density (pressure). It has both positive and negative values<sup>12</sup>. In the case of hydrogen isotopes, chemical potentials are positive only. This means that these isotopes cannot form a mixture with  $^4\text{He}$ . The positive and negative values of chemical potential of  $^3\text{He}$  and  $^4\text{He}$  clearly indicate that we have  $^3\text{He} - ^4\text{He}$  mixtures. The recent estimate of chemical potential of deuterium at saturation density shows that it has positive values<sup>13</sup>.

So far theoretical estimation of chemical potential of liquid  $^3\text{He}$  is concerned, there are few theoretical calculations and none of them is found very satisfactory in explaining the pressure dependence of chemical potential. Recently Mishra and Tripathy<sup>14</sup> have developed a theoretical model for liquid  $^3\text{He}$  in which the liquid is visualised as an interacting system of helium atom and quanta of zero sound mode. This model is able to explain and estimate large number<sup>15-22</sup> of physical properties of liquid  $^3\text{He}$  which are in good agreement with the experimental data<sup>23-27</sup>.

In this paper, we have presented a method of calculating the chemical potential of  $^3\text{He}$  atom in liquid  $^3\text{He}$ . We have used the Mishra and Tripathy<sup>14</sup> model Hamiltonian in this calculation. We have adopted the procedure of Keldin and Prange<sup>28</sup>, in which chemical potential of an electron has been calculated by evaluating the single particle energy at  $p = k_F$ . In the same way, we have taken the effective single particle energy of Mishra and Tripathy and evaluated the energy  $[\epsilon(p)]$  at  $p = 1$  by making it proper dimensionless. It turns out that the chemical potential even at  $p = 0$  is greater than unity. Our calculated result increases with pressure. The model potential used in our calculation is a type of contact interaction, which has been widely used by a large number of workers<sup>29,31</sup>.

**2 Mathematical Formulae Used in the Calculation**

Taking effective single particle energy of Mishra and Tripathy model<sup>14</sup>

$$E_0(k_c) = \langle Y_0 | H_{ncw} | Y_0 \rangle$$

$$= \sum_{ps} \bar{\epsilon}_p n_{ps} - n \sum_{|k| < k_c} v(k)/2 + 1/2 \sum_{|k| < k_c} \Omega_{ph}^{(0)}(k)$$

$$+ \sum_{|k| < k_c} \sum_{p\sigma} r_3(k, p) r_3(-k, p+k) \left\{ \frac{\Omega_{ph}^{(0)}(k)}{\Omega^2(k) - \omega_{pk}^2} \right\}$$

$$n_{p\sigma} (1 - n_{p+k\sigma}) - \sum_{|k| < k_c} \sum_{p\sigma} 1/2 v(k) n_{p\sigma} n_{p+k\sigma} \quad \dots(1)$$

where  $\Omega(k)$  is the renormalized frequency, given by

$$\Omega(k) = [\Omega_{ph}^{(0)2}(k) + 2\Omega_{ph}^{(0)}(k) \text{Re} \pi_0\{k, \Omega_{ph}^{(0)}(k)\}]^{1/2} \dots(2)$$

and

$$\Omega_{ph}^{(0)}(k) = [\Omega_{ph}^{(0)2}(k) + 2\Omega_{ph}^{(0)}(k) \text{Re} \pi_0\{k, \Omega_{ph}^{(0)}(k)\}]^{1/2} \dots(3)$$

and  $\Omega_{ph}^{(0)}(k)$  is the bare phonon frequency in the  $k$ th mode

$$\Omega_{ph}^{(0)}(k) = \left[ \frac{4pb\hbar^2}{m} \right]^{1/2} k \quad \dots(4)$$

$\bar{\epsilon}_p$  is given as

$$\bar{\epsilon}_p = \epsilon_p + \sum_{|k| < k_c} \{r_3(k, p)\}^2 \left[ \frac{\omega_{pk}}{\Omega_{ph}^{(0)2}(k) - \omega_{pk}^2} \right] \dots(5)$$

$$\left[ \begin{aligned} \epsilon_p &= \frac{\hbar^2 p^2}{2m} \\ \omega_{pk} &= (\epsilon_{p+k} - \epsilon_p) \end{aligned} \right] \dots(6)$$

$r_3(k, p)$  is the coupling constant between <sup>3</sup>He atom

and zero – sound quanta

$$r_3(k, p) = \left[ \frac{v(k)}{2\Omega_{ph}^{(0)2}(k)} \right]^{1/2} (\epsilon_{p+k} - \epsilon_p) \quad \dots(7)$$

and model potential<sup>32</sup>  $v(k)$  is

$$v(k) = \frac{4\pi b \hbar^2}{m} \quad \dots(8)$$

where  $b$  is the scattering length of free helium atom ( $b = 2.556 \text{ \AA}$ ).

Using the definition<sup>28</sup> the chemical potential  $\mu_1^{(0)}$  or <sup>3</sup>He atom in liquid <sup>3</sup>He at  $T = 0$  is given by

$$\mu_1^{(0)} = [p^2 + \Sigma(p, p^2)]_p = 1$$

$$= [\epsilon_f(p)]_p = 1 \quad \dots(9)$$

where  $\Sigma(p, p^2)$  denotes the proper self-energy term to  $\epsilon_p = p^2$  in the dimensionless form. This amounts to carrying out of the numerical integration over one-dimensional space for  $p = 1$  for liquid <sup>3</sup>He.

Actually, one has to evaluate the following term

$$[\epsilon_f(p)]_{p=1} = [\epsilon_{f1a}(p) + \epsilon_{f2a}(p) + \epsilon_{f2}(p) + \epsilon_{f3}(p) + \epsilon_{f4}(p) + \epsilon_{f5}(p)]_{p=1} \quad \dots(10)$$

Here  $\epsilon_f(p)$  are the various terms in the rhs of Eq. (1).

Now, various  $\epsilon_f(p)$  in the dimensionless form can be written as

$$[\epsilon_{f1a}(p)]_{p=1} = 3/5 = 0.6 \quad \dots(11)$$

$$[\epsilon_{f1b}(p)]_{p=1} = \{0.16540 \int_0^{\beta} k^3 dk \int_0^1 p^2 dp$$

$$[-2kp + \frac{a_0^2}{4} \log | \frac{a_0^2 - (k-2p)^2}{a_0^2 - (k+2p)^2} | ]\}_{p=1} \quad \dots(12)$$

$$[\epsilon_{r2}(p)]_{p=1} = -0.42633 \beta^3$$

$$[\epsilon_{r3}(p)]_{p=1} = 0.34628 \beta^4$$

$$[\epsilon_{r4}(p)]_{p=1} = \left\{ -1.91847 \int_0^{\beta-1} p^2 \int_{(1-p)}^{(1+p)} k^2 dk \right.$$

$$\left. \int_{\alpha}^1 dx + \int_0^{\beta-1} p^2 dp \int_{(1-p)}^{\beta} k^2 dk \int_{-1}^{+1} dx + \int_{(\beta-1)}^1 p^2 dp \right.$$

$$\left. \int_{(1-p)}^{\beta} k^2 dk \int_{\alpha}^1 dx \left[ \frac{(k^2 + 2pkx)^2}{\Omega^2(k) - (k^2 + 2pkx)^2} \right] \right\}_{p=1} \dots(13)$$

where

$$\Omega^2(k) = a_0^2 k^2 + a_0^2 k^2 \left\{ -1 - \Omega_{ph}^2(k) \left\{ \left( \frac{3}{8} k^2 \right) \right. \right.$$

$$\left. \left. + \frac{3}{16k^3} \left[ \left\{ 1 - \left( \frac{\Omega_{ph}(k) - k^2}{2k} \right)^2 \right\} \ln \left| \frac{\Omega_{ph}(k) - k^2 - 2k}{\Omega_{ph}(k) - k^2 + 2k} \right| \right. \right. \right.$$

$$\left. \left. \left\{ 1 - \left( \frac{\Omega_{ph}(k) + k^2}{2k} \right)^2 \right\} \ln \left| \frac{\Omega_{ph}(k) + k^2 - 2k}{\Omega_{ph}(k) + k^2 + 2k} \right| \right] \right\} \dots(14)$$

and

$$\Omega_{ph}^2(k) = a_0^2 k^2 + a_0^2 k^2 \left\{ -1 - a_0^2 k^2 \left\{ \left( \frac{3}{8} k^2 \right) \right. \right.$$

$$\left. \left. + \frac{3}{16k^3} \left[ \left\{ 1 - \left( \frac{a_0 k - k^2}{2k} \right)^2 \right\} \ln \left| \frac{a_0 k - k^2 - 2k}{a_0 k - k^2 + 2k} \right| \right. \right. \right.$$

$$\left. \left. \left\{ 1 - \left( \frac{a_0 k + k^2}{2k} \right)^2 \right\} \ln \left| \frac{a_0 k + k^2 - 2k}{a_0 k + k^2 + 2k} \right| \right] \right\} \dots(15)$$

where  $a_0 = 1.84685$

$\beta = k_v/k_F = 1.78$

$$\alpha = \left( \frac{1 - p^2 - k^2}{2pk} \right)$$

$$[\epsilon_{r5}(p)]_{p=1} = -0.04447 + 0.0334 \beta \dots(16)$$

Now Eq. (10) is solved for a given value of  $p$  which determines the value of  $a_0$  and  $\beta$ . The calculations have been repeated from pressure  $p = 0 \times 10^5$  Pa to  $P = 21 \times 10^5$  Pa and corresponding values of  $\beta$ ,  $a_0$ ,  $\mu_1(0)$  and  $\mu_1$  have been determined. The results are shown in Table 1-3 respectively. The calculation shows that chemical potential increases with pressure. The present results are in a satisfactory agreement with the experimental data at least for high density<sup>33</sup>. The different contribution to the <sup>3</sup>He impurity chemical potential as a function of density has been given in Table 3.

Table 1 — Various parameters used for contact interaction potential

Pressure $P \times 10^5$ Pa	$k_p$ (nm <sup>-1</sup> )	$v_p$ (m/s)	$\epsilon_p$ (K)	$a_0$ ( $v_p$ )
0	7.85	165.15	4.95	1.84561
3	8.08	169.99	5.24	1.87245
6	8.23	173.14	5.44	1.88975
9	8.34	175.46	5.58	1.90234
12	8.43	172.33	5.70	1.91258
15	8.52	179.24	5.83	1.92276
18	8.60	180.93	5.94	1.93176
21	8.65	181.98	6.01	1.93737

Table 2 — Pressure  $P(10^5$  Pa), density  $\rho$  ( $\text{\AA}^{-3}$ ),  $\mu_0(K)$  and  $\mu_1(0)^{cal}$  (K)

Pressure $P \times 10^5$ Pa	density $\rho$ ( $\text{\AA}^{-3}$ )	$\mu_0$ (K)	$\mu_1(0)$ (K)
0	0.01634	4.95	1.4294
3	0.01782	5.42	1.4738
6	0.01883	5.44	1.5528
9	0.01959	5.58	1.6896
12	0.02023	5.70	1.9353
15	0.02089	5.83	2.0268
18	0.02148	5.94	2.0268
21	0.02186	6.01	3.6257

Table 3 — Different contribution to the  $^3\text{He}$  impurities chemical potential as a function of density<sup>36</sup>

$\rho$ ( $\text{\AA}^{-3}$ )	$\mu_{\text{HNC}}$ (K)	$\mu_{\text{c3}}$ (K)	$\mu_{\text{elem}}$ (K)	$\mu_{\text{total}}$ (K)
0.019	1.65	-2.32	-5.58	-6.25
0.020	4.16	-2.91	-6.49	-5.24
0.021	7.12	-3.61	-7.51	-4.00
0.022	10.60	-4.46	-8.66	-2.52
0.023	14.65	-5.47	-9.95	-0.77
0.024	19.34	-6.67	-11.39	1.27
0.025	24.78	-8.11	-13.01	3.64

### 3 Discussion of Results

A method of calculating pressure dependent chemical potential of  $^3\text{He}$  atom in liquid  $^3\text{He}$  is presented. This method of calculation depends upon the procedure given by Keldin and Prange<sup>28</sup>, in which chemical potential of an interacting system is calculated by evaluating the effective single particle energy  $[\mathcal{E}(p)]$  at  $p = 1$ . The term  $p$  is the momentum transfer in the unit of Fermi momentum  $k_F$ . The results show that chemical potential increases with pressure, which are in satisfactory agreement with the experimental data at least for higher density<sup>33</sup>. For low pressure (density), experimental result indicates negative value of chemical potential for  $^3\text{He}$  impurity, which the present calculation does not show. Mishra and Triparthy<sup>14</sup> model Hamiltonian has been adopted for the evaluation of chemical potential. This model Hamiltonian is found very successful in explaining large physical properties of liquid  $^3\text{He}$ . The results also indicate that chemical potential of interacting system is always greater than unity. This fact is also discussed in the text book on *Statistical Mechanics* by Lifshitz and Pitaevski<sup>34</sup>. Singh and Mishra<sup>20</sup> have recently shown that effective mass ( $m^*/m$ ) varies with pressure by taking increase in chemical potential with pressure in their calculation. Negative value of chemical potential is not shown for low pressure (density) as per experimental observations because the present model potential is a type of contact interaction potential<sup>32</sup>. This interaction potential is totally repulsive in nature having only scattering length parameter  $b$  which varies with density. With a more realistic potential for liquid  $^3\text{He}$ , it may be possible to show the negative chemical potential with this type of formalism. Saarela and Krotschek<sup>35</sup> have evaluated the

chemical potential of  $^3\text{He}$  impurity using extended Jastrow – Feenberg theory based on correlated wave function (HNC). These calculations also indicate that  $\mu_{\text{HNC}}(k)$  increases with increase of density and values are greater than unity. In fact, these values  $[\mu_{\text{HNC}}(k)]$  varies from 1.65 to 24.78 as density increases from 0.019 ( $\rho \text{\AA}^{-3}$ ) to 0.025 ( $\rho \text{\AA}^{-3}$ ). There was also a calculation of chemical potential of  $^3\text{He}$  impurity by Fabrocini *et al.*<sup>36</sup>. They improve the variational wave function by correlated basis functions (C B F) perturbation theory and summed up specific class of diagrams up to infinite order. The elementary class of diagram gives the value of chemical potential  $\mu_{\text{c3}}(k)$  which varies from -5.58 to -13.01 as density varies from 0.019 ( $\rho \text{\AA}^{-3}$ ) to 0.025 ( $\rho \text{\AA}^{-3}$ ). Taking total C B F diagrams into their calculation, it was found that  $\mu_{\text{total}}(k)$  varies from -6.25 to 3.64 as density varies from 0.019 ( $\rho \text{\AA}^{-3}$ ) to 0.025 ( $\rho \text{\AA}^{-3}$ ). The calculations made taking HNC/0 approximations by including elementary diagrams and to improve upon the Jastrow theory by including triplet correlations in the ground state, the chemical potential of  $^3\text{He}$  impurity  $\mu_{\text{c3}}(k)$  also varies from -2.32 to -8.11 against density 0.019 ( $\rho \text{\AA}^{-3}$ ) to 0.025 ( $\rho \text{\AA}^{-3}$ ) respectively. These results are shown in Table 3.

### Acknowledgement

One of the author (LKM) expresses a deep sense of gratitude and sincere thanks to Late Professor D. N. Tripathy, Institute of Physics, Bhubaneswar (Orissa) for his valuable guidance, inspiration and co-operation throughout his life. We are very much thankful to our departmental colleague for their co-operation and help.

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