Regular Article

Calculation of Thermodynamic Properties of the Quasi-one Dimensional Liquid [3]He at Finite Temperature

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We have used a variational approach to calculate some thermodynamic properties of the quasi-one dimensional liquid [3]He such as the energy, entropy, free energy, equation of state and heat capacity at finite temperature. We have employed the Lennard-Jones potential as the inter-atomic interaction. We have seen that the total energy increases by increasing both temperature and density. As expected, it is seen that the entropy decreases by increasing density and decreasing temperature. There is no minimum point in the free energy curve, showing that there is not any bond state for the quasi-one dimensional liquid [3]He. The results of our calculations indicate that the equation of state of this system becomes stiffer as the temperature increases. Our results for the specific heat show that there is not any lambda transition for this system.

Keywords: Liquid [3]He, Quasi-one dimension, Thermodynamic properties

INTRODUCTION

Helium has two stable isotopes, one with mass number 4 and the other with mass number 3. The first one is available as helium gas or liquid from the atmosphere or gas wells, while the second one is extremely rare in nature and has bean only available commercially since 1950 [1].

Liquid [3]He is particularly suited to study the correlation among the strongly interacting many-body fermionic systems. Several approaches have been used for investigating the properties of liquid [3]He. These are mainly based on the Singwi, Tosi, Land and Sjölander (STLS) scheme [2], mott localization [3], spin fluctuation theory [4], Green's function Monte Carlo (GFMC) [5], nonperturbative renormalization group equation [6], nonlocal density functional formalism [7], correlated basis functions CBF [8], and Fermi hyper-netted chain (FHNC) [9]. Recently, a Japanese group have verified [3]He atoms in a narrow tube at zero temperature applying the Monte Carlo method [10]. They have calculated the ground state energy

of this system at zero temperature for the cases in which the tube has the radius of order 1 nm.

In recent years, we have studied the bulk properties of the normal and polarized [3]He at zero and finite temperatures [11-21]. In these calculations, the lowest order variational method based on the cluster expansion of the energy functional has been used. This method is fully self-consistent, since it does not introduce any free parameter to the calculations. Very recently, we have used the lowest order variational method to calculate some ground state properties of two-dimensional liquid [3]He at zero temperature [22].

In the present work, we study the quasi-one dimensional liquid [3]He. Quasi-one dimensional liquid [3]He system can be produced by injecting the [3]He atoms into a nanotube. Here, we intend to calculate some thermodynamic properties of this system at finite temperature using a variational method employing the Lennard-Jones pair potential [23].

Method

Our quasi-one dimensional system contains [3]He atoms confined in a very long cylinder with radius about $a = 10$

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nm. Our calculations have been carried out for the number density (number of particles per unit length, $\rho = N/L$) in the range 0.001-0.01 nm^{-1} at the temperatures in the range 1.0-4.0 K. For computing the thermodynamic properties of such a system, first we must calculate its internal energy. For this purpose, we use the lowest order variational method.

Lowest Order Variational Method Formalism

The lowest order variational method is a variational many-body technique based on the cluster expansion of the energy functional [24],

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = E_1 + E_2 + ..., \tag{1}$$

where E_1 is the one-body cluster energy, E_2 is the two-body cluster energy, and *etc*. We consider the energy of the system up to the second term in the cluster expansion, and ignore the higher order terms [25].

The one-body energy is as follows,

$$E_1 = \sum_k n(k)\varepsilon(k), \tag{2}$$

where

$$n(k) = \frac{1}{e^{\beta(\varepsilon(k)-\mu)}+1}, \tag{3}$$

is the Fermi-Dirac distribution function. In the above equation, $\varepsilon(k)$ is the single particle energy, $\beta = 1/k_BT$ and μ is the chemical potential. For each density and temperature, the chemical potential can be obtained using the following constraint,

$$N = \sum_k \frac{1}{e^{\beta(\varepsilon(k)-\mu)}+1}. \tag{4}$$

The two-body energy has the following form,

$$E_2 = \frac{1}{2}\sum_{i,j}\langle ij | \omega(12) | ij - ji \rangle, \tag{5}$$

where

$$\omega(12) = \frac{\hbar^2}{m}[\nabla f(r)]^2 + f^2(r)V(r). \tag{6}$$

In the above equation, $V(r)$ is the inter-particle potential and $f(r)$ is the two-body correlation function.

Lowest Order Variational Method Calculations for Quasi-one Dimensional Liquid ^{3}He

Now, we are going to obtain the energy of quasi-one dimensional liquid ^{3}He using the relations introduced in the above section.

To calculate the one-body energy (E_1), we use Eq. (2) in which the single particle energy ($\varepsilon(k)$) for the cylindrical coordinates is approximately written in terms of effective mass, as follows

$$\varepsilon(k) = \frac{\hbar^2}{2m^*}[(\frac{X_{10}}{a})^2 + k^2], \tag{7}$$

where a is the radius of cylinder, $k = \pi v/L$ is the single particle wave vector, and X_{10} is the first root of J_0 (J_0 is the zeroth order Bessel function) [26]. Here, v is the quantum number corresponding to the energy eigenvalue. In fact, we use a quadratic approximation for single particle potential incorporated in the single particle energy as a momentum independent of effective mass. We introduce the effective mass, m^*, as a variational parameter [27].

For calculating the two-body energy, we use Eq. (5). Since we intend to calculate the energy of quasi-one dimensional liquid ^{3}He, we consider the following single particle wave function for the system, which is the result of Schrödinger equation for a cylindrical box,

$$\langle \vec{r} | i \rangle = AJ_0(\gamma_{10}\rho)sin(vz), \tag{8}$$

Where ρ and z are cylindrical coordinates, A is the normalization factor, and $\gamma_{10} = X_{10}/a$. By inserting Eq. (8) into (5), and doing some algebra, we get the following relation for the two-body energy per particle,

$$E_2 = \frac{(2.4\times10^{-5})}{N}\iint d^3r_1 d^3r_2 J_0^\dagger(\gamma_{01}\rho_1)J_0^\dagger(\gamma_{01}\rho_2)J_0(\gamma_{01}\rho_1)J_0(\gamma_{01}\rho_2)$$

$$\times \omega(12)\sum_{k_i k_j}n(k_i)n(k_j)\sin(k_iz_1)\sin(k_jz_2)$$

$$\times [2\sin(k_iz_1)\sin(k_jz_2) - \sin(k_jz_1)\sin(k_iz_2)]. \tag{9}$$

To calculate the two-body energy, at first, we must compute

ω(12) (Eq. (6)). Here, we employ the Lennard-Jones potential [23] as the helium-helium interaction,

$$V(r) = 4\varepsilon[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6}], \qquad (10)$$

where $\varepsilon = 10.22$ k and $\sigma = 0.2556$ nm. We also consider the following two-body correlation function,

$$f(r, \rho, T) = 1 - e^{-\alpha r^2}, \qquad (11)$$

where $\alpha = \alpha(\rho, T)$ is a density and temperature dependent form variational parameter. We have chosen this correlation function because when r goes to zero, the correlation function should approach to zero and when r goes to infinity, the correlation function should approach to unity. For each value of density and temperature, we minimize the two-body energy with respect to the variation in the α parameter.

Finally, thermodynamic properties of the system is obtained from the free energy, $F = E - TS$, where

$$S = -k_B \sum_k [(1 - n(k)) \ln(1 - n(k)) + n(k) \ln(n(k))], \qquad (12)$$

is the entropy of system. As mentioned in the previous section, the effective mass has been considered as a variational parameter. Therefore, we minimize the free energy with respect to the variation in the effective mass, then we obtain the chemical potential and the effective mass. This minimization is carried out numerically.

RESULTS AND DISCUSSIONS

We have shown the one-body energy per particle (E_1) *vs.* density in Fig. 1 for various temperatures (1.0-4.0 K). As seen, E_1 increases by increasing both density and temperature. However, this energy is more sensitive to the variation of temperature. From our numerical results, it is found that the slope of energy curve decreases as the temperature increases.

In Fig. 2, we have plotted the two-body energy per particle (E_2) as a function of density at $T = 1.0$-4.0 k. We can see that the interaction energy increases by increasing the density, while it decreases by increasing the temperature. The total energy per particle ($E = E_1 + E_2$) has been shown in Fig. 3. We see that the total energy increases by increasing both density and temperature. Here, we can
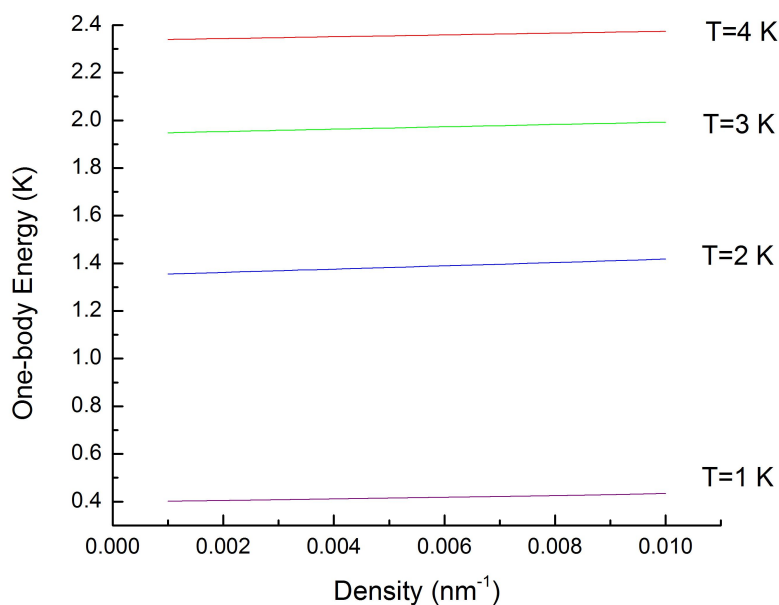

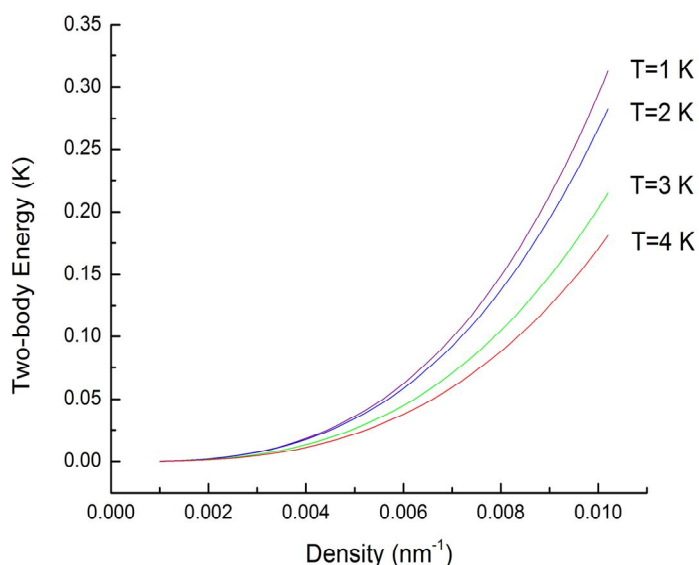**Fig. 1.** One-body energy per particle *vs.* density at different temperatures (*T*).

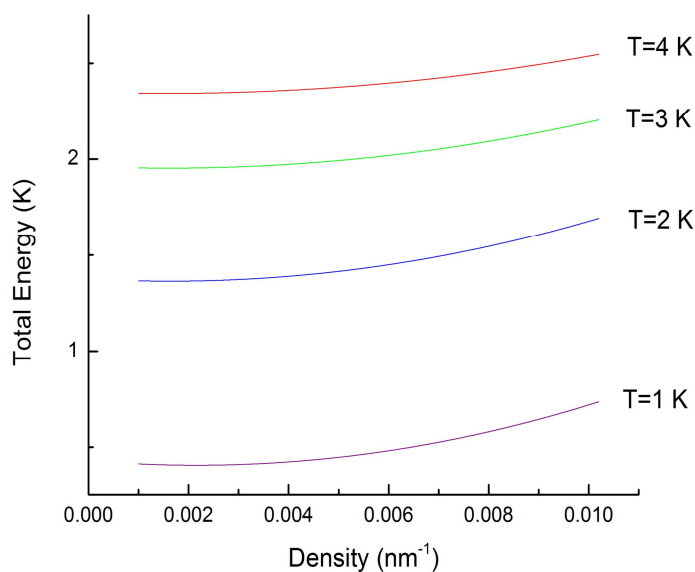**Fig. 2.** Two-body energy per particle *vs.* density at different temperatures (*T*).

Fig. 3. Total energy per particle *vs.* density at different temperatures (*T*).

conclude that the increasing of one-body energy (E_1) by temperature (Fig. 1) dominates the decreasing of two-body energy (E_2) by temperature (Fig. 2), leading to the increase of total energy by increasing the temperature.

Using Eq. (12), we can find the entropy per particle for the system. In Fig. 4, the entropy versus density has been presented at different temperatures. As known, for any system, the entropy should be reduced by increasing the density, and increased by increasing the temperature [28]. Figure 4 shows that this is consistent with our result.

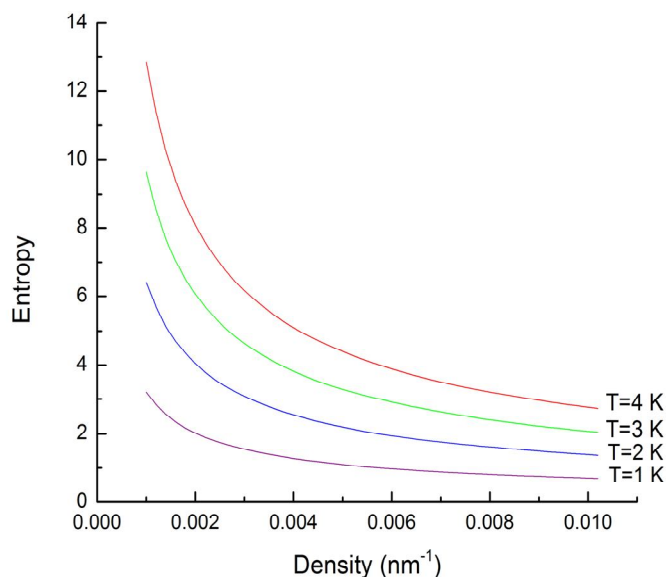The free energy per particle versus density for various temperatures (1.0-4.0 K) has been shown in Fig. 5. This

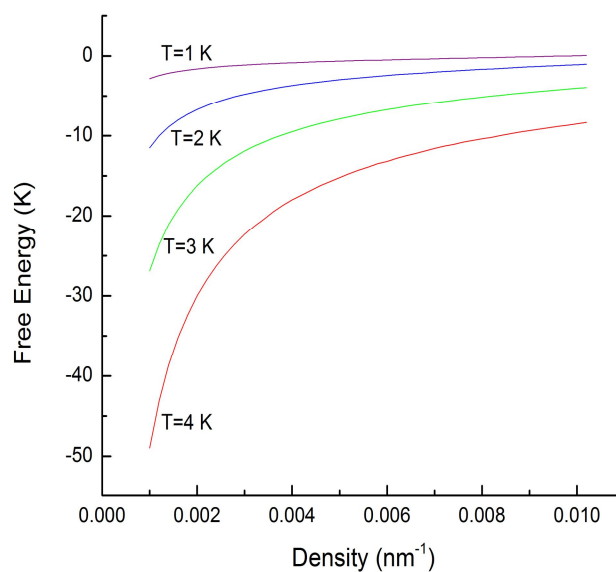**Fig. 4.** Entropy per particle *vs*. density at different temperatures (*T*).

Fig. 5. Free energy per particle *vs*. density at different temperatures (*T*).

figure shows that free energy increases by increasing the density, while it decreases by increasing the temperature, especially at low densities. We also see that there is no minimum point in the free energy curve. This indicates that there is no bond state for this system. As seen from Fig. 5, at low densities, the free energy increases very rapidly by density, especially at higher temperatures. As seen from Figs. 3 and 4, at a fixed temperature, by increasing the density, the internal energy increases, while the entropy decreases, therefore this leads to the increasing of free energy by increasing the density. This behavior of free energy is very considerable at low densities.
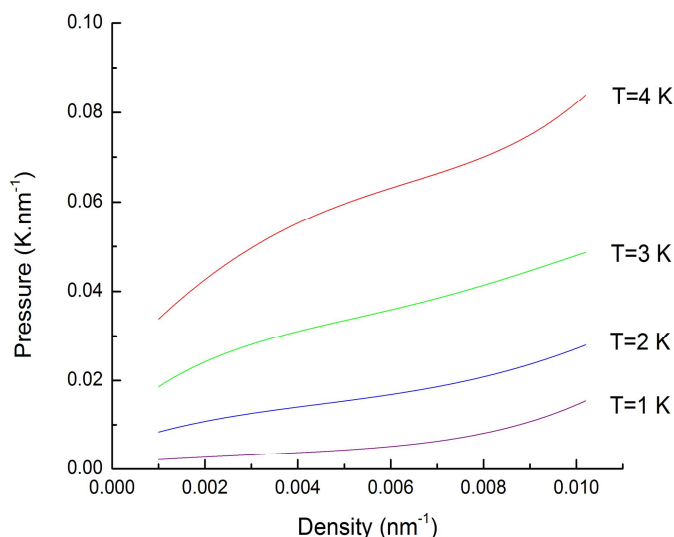
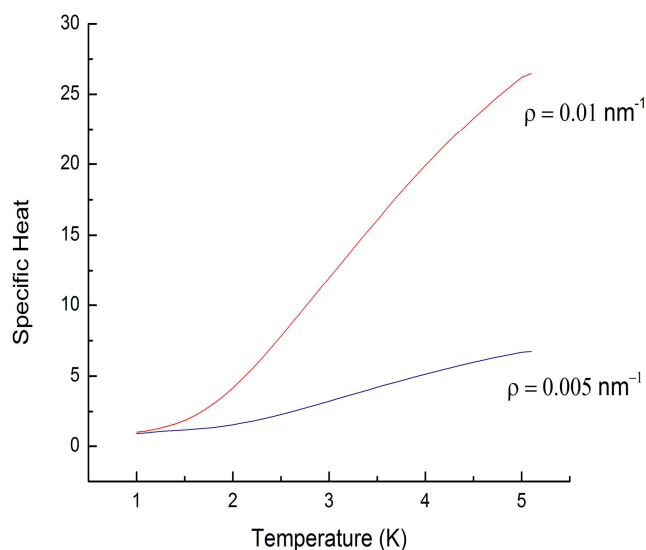**Fig. 6.** Pressure *vs.* density at different temperatures (*T*).

Fig. 7. Specific heat *vs.* temperature for different densities (*ρ*).

Now, we are in a position to find the pressure of the system using the following relation,

$$P = \rho^2 \frac{\partial F}{\partial \rho}. \tag{13}$$

In Fig. 6, we have presented the pressure of the system versus density (equation of state) for temperatures (1.0-4.0 K). We see that the pressure increases by increasing both density and temperature. This indicates that the equation of state of system becomes stiffer as the temperature increases. We also see that the difference of pressure for different temperatures is substantial at high densities.

Finally, we have calculated the specific heat at constant

volume (C_v) of our system from the internal energy,

$$C_v = (\frac{\partial E}{\partial T})_v.$$ (14)

We have given the specific heat versus temperature for two values of density ($\rho = 0.005$ and 0.01 nm^{-1}) in Fig. 7. This figure shows that the specific heat increases by increasing both temperature and density. We know that a fermionic system does not have a lambda transition in its specific heat diagram, and the specific heat should increase by increasing the density for such a system. Figure 7 shows that our results obey this physical criteria. We also see that as the temperature approaches zero, the specific heat for all densities goes to zero.

SUMMARY AND CONCLUSIONS

In this paper, we have considered a quasi-one dimensional liquid ^{3}He at finite temperature. Our system contains N ^{3}He atoms confined in a very long cylinder with radius 10 nm. Thermodynamic properties of this systen have been verified using the variational method based on the cluster expansion of energy. First, we have calculated the one-body (E_1) and the two-body (E_2) energies, then the total energy ($E = E_1 + E_2$) has been obtained. Our results show that the one-body energy increases by increasing both temperature and density, while the two-body energy increases by density,and decreases by increasing temperature. The total energy has a similar behavior with one-body energy (E_1). In fact increasing of one-body energy by temperature dominates the decreasing of two-body energy by temperature. We have also calculated entropy of the system, which increases by temperature and decreases by density. It is found that the free energy increases by density and decreases by temperature. We also see that there is no minimum point on the free energy curve which means that there is not any bond state for the system. We have computed the equation of state for the system, showing that the equation of state becomes stiffer as the temperature increases. Here, the specific heat at constant volume has been also calculated. Our results do not show any lambda transition for the quasi-one dimensional liquid ^{3}He.

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