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Isentropic calculations for normal liquid ^3He using the lowest order constrained variational method

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Abstract

In this paper the lowest order constrained variational (LOCV) method has been used for calculation of liquid ^3He along different isentropic paths employing the Aziz potential. Some thermodynamic properties such as energy per particle, pressure, temperature, chemical potential, velocity of sound, adiabatic index and compressibility for normal liquid ^3He have been calculated. Our results indicate that the sound velocity is always less than the velocity of light in vacuum (c) showing that all calculated equations of state obey the causality condition. Finally, our calculations show that the adiabatic index is not constant and its value depends on both density and entropy of the system.

Keywords: Liquid ^3He; isentropic process; velocity of sound; adiabatic index; compressibility

1. Introduction

Helium 3 is one of the two stable isotopes of helium (^3He and ^4He) [1]. The quantum natures of the two isotopes of helium are qualitatively different. ^4He atoms behave as an ideal Bose gas whose properties are described by Bose-Einstein statistics, while the ^3He atoms behave as an ideal Fermi gas with properties described by Fermi- Dirac statistics. Liquid ^3He changes from a classical to a quantum liquid as it is cooled to the millikelvin region and it forms a liquid having the lowest known boiling point of $3.19\ K$ and only solidifies under the pressure of $3.45\ Mpa$.

Different many-body techniques have been used for investigating the properties of liquid ^3He. These calculations are mainly based on the Green's function Monte Carlo (GFMC) [2], FN-DMC, DMC, VMC and EMC simulations [3-6], correlated basis functions (CBF) [7, 8] and Fermi hyper-netted chain (FHNC) [9-13]. In this article, we use the lowest order constrained variational (LOCV) method in the calculations for normal liquid ^3He.

The LOCV method which is based on the cluster expansion of the energy functional, has been developed to study the bulk properties of the quantal fluids [14-16].

In our previous papers, by employing the LOCV method, we have calculated some properties of the normal and polarized liquid ^3He at finite temperature with the spin-independent correlation function [17-19]. We have also studied polarized liquid ^3He with the spin-independent and spin-dependent correlation function at zero temperature [20-22]. These calculations have been also extended for the normal and polarized liquid ^3He in the case of spin-dependent correlation function at finite temperatures [23, 24].

The LOCV method has several advantages with respect to the other many-body formalisms. This is a fully self-consistent method and does not introduce any free parameter to the calculations. The crucial point in this method is the functional minimization with respect to the two-body correlation function subjected to the normalization constraint which finally leads to the Euler-Lagrange differential equation. The convergence of its results has been shown by computing the three-body cluster energy term [22, 25].

In this article, the LOCV method is used to compute the thermodynamic properties of normal liquid ^3He along the isentropic paths with the spin-independent correlation function employing the Aziz potential.

2. Lowest Order Constrained Variational Method

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We consider a system of N interacting ^3He atoms. For this system, the Fermi-Dirac distribution function is [26].

$$n(k,S,\rho)=\frac{1}{e^{\beta[\varepsilon(k,S,\rho)-\mu(S,\rho)]}+1}\cdot \quad (1)$$

In the above equation $\beta=\frac{1}{k_BT}$, μ is the chemical potential, ρ is the number density and ε is the single particle energy of a ^3He atom. In our formalism, the single particle energy, ε,of a ^3He atom with momentum k is approximately written as

$$\varepsilon(k,S,\rho)=\frac{\hbar^2k^2}{2m}+U(S,\rho). \quad (2)$$

$U(S,\rho)$ is the momentum independent single particle potential. The chemical potential, μ, and the temperature, T, at any adopted values of the entropy (S) and the number density (ρ), are determined by applying the following constraints,

$$N=\sum_k n(k,S,\rho) \quad (3)$$

$$S=-k_B\sum_k \{[1-n(k,S,\rho)]\, ln[1-n(k,S,\rho)]+n(k,S,\rho)lnn(k,S,\rho)\}. \quad (4)$$

These are implicit equations which can be solved numerically.

To calculate the energy of this system we consider up to the two-body term in the cluster expansion of the energy functional [27],

$$E(S,\rho)=E_1(S,\rho)+E_2(S,\rho) \quad (5)$$

where

$$E_1(S,\rho)=\ \frac{\hbar^2}{2\pi^2m\rho}\int_0^\infty n(k,S,\rho)k^4dk \quad (6)$$

and

$$E_2(S,\rho)=\frac{1}{2N}\sum_{ij}\langle ij|W(12)|ij-ji\rangle \quad (7)$$

In the above equation, $W(12)$ is

$$W(12)=\frac{\hbar^2}{M}[\nabla f(12)]^2+f(12)V(12)f(12), \quad (8)$$

where $V(12)$ is the two-body potential and $f(12)$ is the two-body correlation operator. After some calculations, the following final expression for the two body energy $E_2(S,\rho)$ has been derived.

$$E_2(S,\rho)\ \frac{\hbar^2\rho^2}{2m}\int_0^\infty [(f'(r))^2+\frac{m}{\hbar^2}f^2(r)V(r)]a^2(r,S,\rho)r^2dr, \quad (9)$$

where

$$a^2(r,S,\rho)=1-\frac{1}{2}(\frac{\gamma(r,S,\rho)}{\rho})^2\cdot \quad (10)$$

In the above equation $\gamma(r,S,\rho)$ is as follows,

$$\gamma(r,S,\rho)=\frac{1}{\pi^2}\int_0^\infty \frac{sinkr}{kr}n(k,S,\rho)k^2dk. \quad (11)$$

We impose the normalization constraint on the two-body correlation function. This means that the correlation function is required to heal to the Pauli function $f_p(r,S,\rho)$ [25],

$$f_p(r,S,\rho)=[1-\frac{1}{2}(\frac{\gamma(r,S,\rho)}{\rho})^2]^{-\frac{1}{2}}\cdot \quad (12)$$

Now, we minimize $E_2(S,\rho)$ with respect to the variation in the correlation function. This gives us the following Euler- Lagrange differential equation

$$g''(r,S,\rho)-[\frac{a''(r,S,\rho)}{a(r,S,\rho)}+\frac{m}{\hbar^2}(V(r)\lambda)]g(r,S,\rho)=0, \quad (13)$$

(2)

where

$$g(r,S,\rho)=f(r,S,\rho)a(r,S,\rho)\cdot \quad (14)$$

λ is the Lagrange multiplier. In the above equations, primes mean differentiation with respect to r. The two-body correlation function is obtained by numerically integrating Eq. (13), the energy per particle of the system can be determined afterwards. Now by calculating $E(S,\rho)$, we can calculate the thermodynamic properties of normal liquid ^3He along different isentropic paths.

3. Results and discussion

The internal energy per particle for the normal liquid ^3He as a function of density along six different constant entropy paths ($S=1.0$, 1.5, 2.0, 2.3, 2.4, and 2.5 k_B) has been shown in Fig. 1. In this Fig., it is seen that for all densities, the internal energy increases by increasing the entropy. It is also shown that at high densities the difference between the energies of different isentropic paths decreases. We have found that the internal energy shows a minimum at some entropies. Minimum point in the plot of internal energy versus density for any entropy, shows density where the system is stable (equilibrium state). When liquid ^3He is in equilibrium state, the mean free path between the He atoms is such that, these atoms are bound together, due to the negative potential energy. However, this minimum disappears for the entropies greater than $S;2.3\ k_B$. We can conclude that for the entropy less than 2.3 k_B, the system at a certain density shows a bound state. Table 1 shows the internal energy at the minimum point (saturation energy) and the corresponding density (saturation density) at different entropies. This table shows that the saturation energy increases by increasing the entropy.

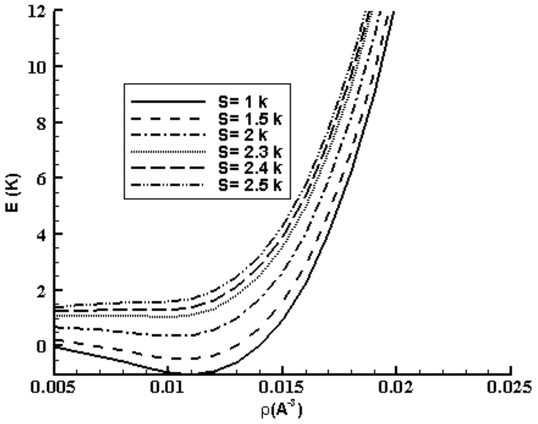

Fig. 1. Internal energy per particle (E) for the normal liquid ^3He as a function of density (ρ) at $S = 1.0$, 1.5, 2.0, 2.3, 2.4 and 2.5 k_B

Table 1. The saturation energy (E_0) and saturation density (ρ_0) for the normal liquid ^3He along different isentropic paths

$S(k_B)$	$\rho_0(A^{-3})$	$E_0(K)$
1.0	0.011	-1.016
1.5	0.011	-0.481
2.0	0.010	0.353

Figure 2 shows the temperature (T) of normal liquid ^3He as a function of density for different values of entropy. From this Fig. it is seen that the temperature increases by increasing both density and entropy. We can see that the rate of increasing temperature versus density increases by increasing the entropy.

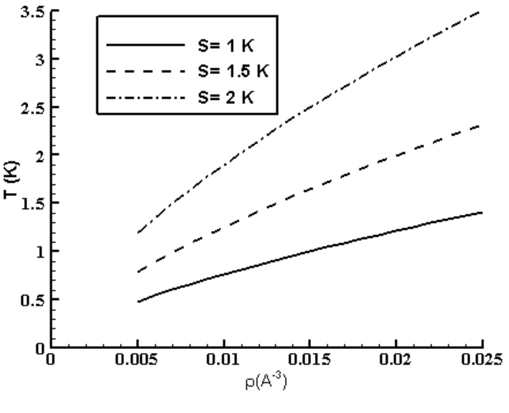

Fig. 2. Temperature (T) of normal liquid ^3He as a function of density (ρ) at $S = 1.0$, 1.5 and 2.0 k_B

The chemical potential (μ) of normal liquid ^3He as a function of density along three constant entropy paths has been presented in Fig. 3. This Fig. indicates that the chemical potential increases (decreases) by increasing density (entropy).

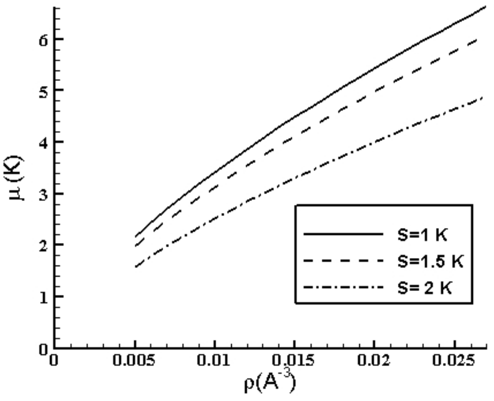

Fig. 3. Chemical potential (μ) of normal liquid ^3He as a function of density (ρ) at $S = 1.0$, 1.5 and $2.0k_B$

The pressure (P) can be obtained from the energy per particle, E, using the following relation,

$$P = \rho^2 \frac{\partial E}{\partial \rho}\bigg|_S . \tag{15}$$

We have drawn our results for the pressure of normal liquid ^3He versus density at different entropies in Fig. 4. In this Fig., it is seen that the pressure is zero for the saturation density (stable state), and nonzero everywhere else. We have found that the pressure increases by increasing both density and entropy. It is seen that at high densities, the increasing of pressure by increasing the entropy becomes faster. Our results show that as the entropy increases, the equation of state of normal liquid ^3He becomes stiffer.

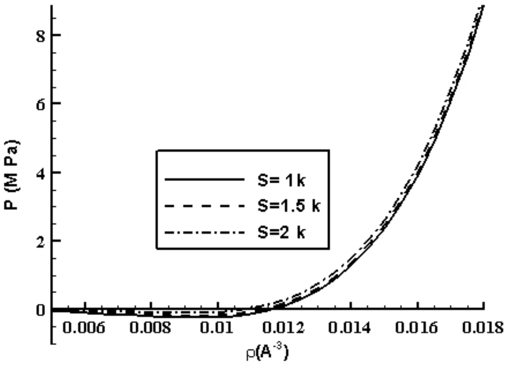

Fig. 4. Pressure (P) of normal liquid ^3He as a function of density (ρ) at $S = 1.0$, 1.5 and 2.0 k_B

One of the interesting parameters in the isentropic process, which checks the obeying causality condition by equations of state, is the velocity of sound (V_s). It can be expressed as

$$V_s = \left[\sqrt{\frac{\partial P}{\partial \rho}}\,\right]_S , \tag{16}$$

where $\rho' = \frac{mN}{V}$ is the mass density and m is the atomic mass of ^3He atom [28]. In Fig. 5, we have plotted V_S for normal liquid ^3He as a function of the density for $S = 1.0$, 1.5 and 2.0 k_B. This Fig. shows that the velocity of sound increases with increasing both density and entropy. However, it is seen that for densities less than about $0.023\ A^{-3}$, V_S for different values of entropies are nearly identical.

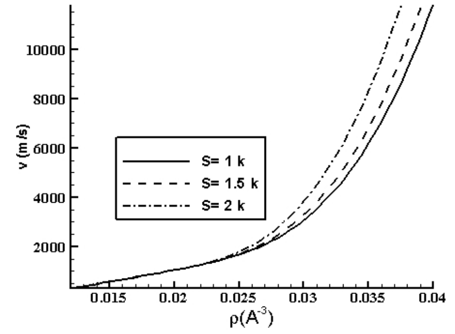

Fig. 5. Velocity of sound (V_S) in the normal liquid ^3He as a function of density (ρ) at $S = 1.0$, 1.5 and $2.0k_B$

Our results for the velocity of sound in the normal liquid ^3He versus pressure at different entropies have been shown in Fig. 6. It is seen that the velocity of sound increases by increasing the pressure. Our results show that for a specific value of pressure, V_S decreases by increasing the entropy. However, from both Figs. 5 and 6, we see that V_S is always less than the velocity of light in vacuum (c). Therefore, we can conclude that all calculated equations of state obey the causality condition. In Fig. 6, our results for the velocity of sound have also been compared with the experimental results [1]. These experimental results show V_S as a function of pressure at finite $T = 0.1\ K$ which is relevant to low densities in our calculations. We can see that in this range our results for velocity of sound are in overall agreement with those of the experiment [1].

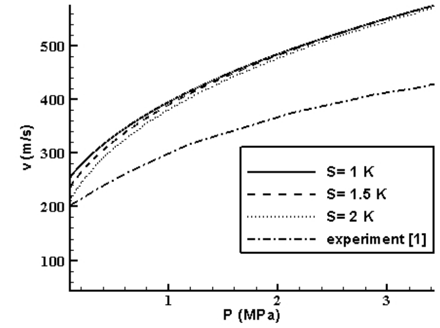

Fig. 6. Velocity of sound (V_S) in the normal liquid ^3He as a function of pressure (P) at $S = 1.0$, 1.5 and 2.0 k_B. The experimental results [1] (dashed dotted) have also been given for comparison.

In Fig. 7, we have compared our results for the velocity of sound in the normal liquid ^3He versus temperature with those of the experiment for $P = 0.1\ MPa$ [29, 30]. We can see that there is an overall agreement between our results and the experimental data, especially at higher temperatures.

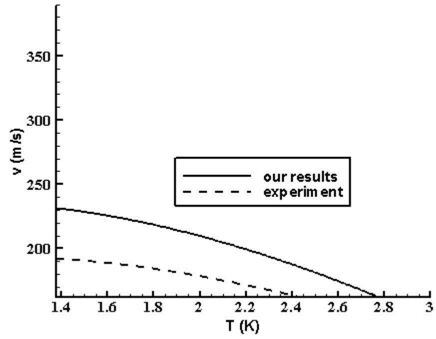

Fig. 7. Velocity of sound (V_S) in the normal liquid ^3He as a function of temperature (T) at $P = 0.1\ MPa$. The experimental results [29, 30] (dashed) have been shown for comparison.

Another interesting parameter in the isentropic calculations is the adiabatic index, Γ, which can be calculated using the following equation:

$$\Gamma = \frac{\rho}{P}\left(\frac{\partial P}{\partial \rho}\right)_S . \qquad (17)$$

Figure 8 shows the adiabatic index for normal liquid ^3He as a function of density at $S = 1.0$, 1.5 and 2.0 k_B. From this figure, it can be found that unlike the ideal gas model, Γ does not have a constant value. We can conclude that this is due to the interactions between the helium atoms in the system. In this Fig. it can be seen that for densities less than about $0.022A^{-3}$, the adiabatic index decreases by increasing both density and entropy. However, for densities greater than about $0.022A^{-3}$, the adiabatic index increases by increasing both density and entropy. Note that as the entropy increases, the minimum point of Γ decreases.

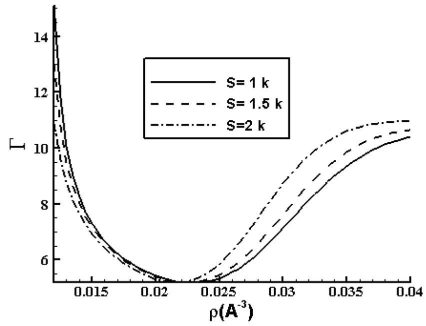

Fig. 8. Adiabatic index (Γ) of normal liquid ^3He as a function of density (ρ) at $S = 1.0$, 1.5 and $2.0k_B$

The isentropic compressibility can be obtained from the following relation,

$$\beta_S = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_S, \qquad (18)$$

where $V = \frac{V}{N} = \frac{1}{\rho}$ [30]. In Fig. 9, we have plotted the isentropic compressibility of normal liquid ^3He as a function of the density for different values of entropy. From this Fig. we can see that the compressibility of normal liquid ^3He decreases by increasing the density. This Fig. shows that for a certain value of density, the compressibility of different entropies are nearly constant.

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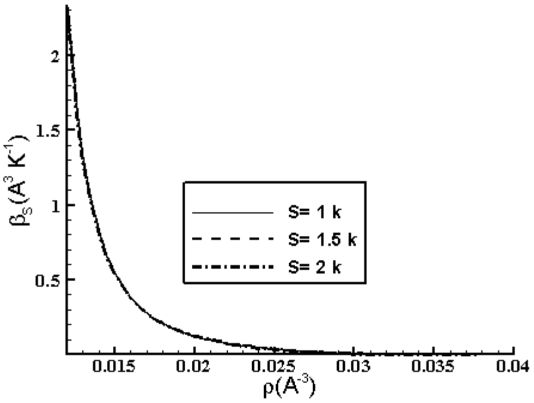

Fig. 9. Isentropic compressibility (β_S) of normal liquid ^3He as a function of density (ρ) at $S = 1.0$, 1.5 and 2.0 k_B

4. Summary and Conclusions

In this work, some thermodynamic properties of liquid ^3He along different isentropic paths using the lowest order constrained variational (LOCV) method were calculated. The Aziz potential was employed in our calculations. It is seen that for all densities, the internal energy increases by increasing the entropy. We have found that the minimum point of energy (saturation energy) increases by increasing the entropy, and it disappears for the entropies greater than about 2.3 k_B. It can be concluded that for the entropies less than about 2.3 k_B, the system at a certain density shows a bound state. We have shown that the pressure and temperature of normal liquid ^3He, as well as the velocity of sound in normal liquid ^3He increases by increasing both density and entropy. It is shown that the velocity of sound in the normal liquid ^3He increases (decreases) by increasing the pressure (entropy and temperature). However, the velocity of sound is always less than the velocity of light in vacuum (c). Therefore, we can conclude that all calculated equations of state obey the causality condition. Our results show that the chemical potential increases by increasing density and decreases by increasing entropy. Our calculations indicate that in spite of the ideal gas model, the adiabatic index does not have a constant value; this is due to the interactions between helium atoms in the system. We have indicated that for densities less (greater) than about $0.022\ A^{-3}$, the adiabatic index decreases (increases) by increasing both density and entropy. Finally, it is seen that the compressibility of normal liquid ^3He decreases by increasing the density, and for a specific value of density, the compressibility remains nearly constant with increasing the entropy.

Acknowledgments

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