

Thermodynamic Properties of Polarized Liquid ^3He along Different Isentropic Paths

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The dependence of some thermodynamic properties of spin-polarized liquid ^3He such as the velocity of sound, adiabatic index, isentropic compressibility and temperature on the spin polarization has been investigated along different isentropic paths. The Lennard-Jones potential has been used in our calculations. It has been found that for higher values of entropy, the spin polarization has greater effect on velocity of sound and adiabatic index with respect to those of lower entropies. Also for a certain value of entropy and density, the isentropic compressibility is almost insensitive to the variations in polarization.

Keywords: Polarized liquid ^3He , Isentropic paths, Correlation function, Velocity of sound, Adiabatic index

INTRODUCTION

The liquid form of the rare isotope of helium, ^3He , has been available only since around 1950, when enough of it was produced by the decay of the tritium manufactured in nuclear reactors. Afterwards, knowledge of the thermodynamic properties of liquid ^3He as strongly correlated many-body fermions has been one of the most interesting in science, specially in condensed matter physics [1]. In recent years, applications of ^3He as a refrigerant, and for other technical purposes have accelerated interests in its thermodynamic properties, particularly in the liquid phase [2]. There are various theoretical methods that are used to study the thermodynamic properties of strongly correlated systems and specially to study the properties of liquid ^3He , such as Green Function Monte Carlo method (GFMC) [3], Fixed Node Diffusion Monte Carlo (FN-DMC), Dynamic Monte Carlo (DMC), Variational Monte Carlo (VMC) and Ensemble Monte Carlo (EMC) simulations [4,5,6,7], correlated basis functions (CBF) [8,9] and Fermi hyper-netted chain (FHNC) [10,11,12,13,14]. Also in recent years, we have done some investigations on both unpolarized and

polarized liquid ^3He at zero and finite temperatures [15,16,17,18,19,20,21,22]. In many of these earlier theoretical works, the thermodynamic properties of liquid ^3He have been studied only in the isothermal process while for each strongly correlated system like liquid ^3He , there are some properties such as velocity of sound, adiabatic index and isentropic compressibility which are needed to be measured along isentropic paths. However, as far as we know, these parameters have been studied mostly by some experimental investigators [23,24,25,26]. Moreover, few theoretical researches on some special properties of liquid ^3He such as velocity of sound and isentropic compressibility have been done only for zero temperature [4,27], and calculation for liquid ^3He at finite entropy has not been done yet. Furthermore, some research such as the studies on the well known so-called Pomeranchuk effect [28] and recent reports on the novel anomalous isentropic effect in a spin mixture of attractively interacting fermionic atoms in an optical lattice [29] show the importance of isentropic investigations for the fermionic systems.

For an interacting many-particle system, the isentropic calculation is a crucial key to obtain some special thermodynamic properties of the system such as the velocity of sound, adiabatic index and isentropic compressibility.

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Recently, we have done some calculations for the unpolarized liquid ^3He along different isentropic paths [30]. In present work, we intend to extend our calculations for the polarized case of liquid ^3He at various entropies. We also investigate the effects of polarization on isentropic properties of this interacting system. In our calculations, we use the variational method employing the Lennard-Jones inter-atomic potential.

ISENTROPIC CALCULATION FOR THE SPIN POLARIZED LIQUID ^3He

Computation of the Chemical Potential and Temperature

The spin polarized liquid ^3He includes $N^{(+)}$ spin-up and $N^{(-)}$ spin-down interacting atoms. For this system, we define the total number density by ρ and the spin asymmetry parameter (spin polarization) by ξ ,

$$\rho = \rho^{(+)} + \rho^{(-)} \quad (1)$$

$$\xi = \frac{\rho^{(+)} - \rho^{(-)}}{\rho^{(+)} + \rho^{(-)}}, \quad (2)$$

where $\rho^{(+)}$ and $\rho^{(-)}$ are the number densities of spin-up and spin-down atoms, respectively. For this polarized system, the spin-up and spin-down atoms have different chemical potentials ($\mu^{(\pm)}$) and different Fermi-Dirac distribution functions, given by [31],

$$n^{(\pm)}(k, S, \rho, \xi) = \frac{1}{e^{\beta[\varepsilon(k) - \mu^{(\pm)}(S, \rho, \xi)]} + 1}, \quad (3)$$

where $\beta = \frac{1}{k_B T}$ and S is the entropy.

For the isentropic calculations, according to the fixed entropy and total number of atoms, we have the following constraints,

$$N^{(\pm)} = \sum_k n^{(\pm)}(k, S, \rho, \xi), \quad (4)$$

$$S = S^{(+)} + S^{(-)} \quad (5)$$

where

$$S^{(\pm)} = -k_B \sum_k \{ [1 - n^{(\pm)}(k, S, \rho, \xi)] \ln [1 - n^{(\pm)}(k, S, \rho, \xi)] \quad (6)$$

$$+ n^{(\pm)}(k, S, \rho, \xi) \ln n^{(\pm)}(k, S, \rho, \xi) \}. \quad (7)$$

We can determine the chemical potentials ($\mu^{(\pm)}$) and the temperature (T), through numerically solving above equations for each value of entropy and number density, ($\mu^{(\pm)}$) (T).

Calculation of the Energy

For calculating the thermodynamic properties of the system, at first we must calculate its energy,

$$E = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \quad (8)$$

By introducing a generalized normalization integral, $I(\alpha)$,

$$I(\alpha) = \langle \psi | \exp[\alpha(H - E_1)] | \psi \rangle, \quad (9)$$

we get the following equation for the energy of system,

$$E = E_1 + \frac{\partial}{\partial \alpha} \ln I(\alpha) \Big|_{\alpha=0}, \quad (10)$$

where α is a parameter and E_1 is the energy of N non-interacting particles. Now, we choose a trial many-body wave function Ψ as follows [32,33],

$$\Psi(1, 2, \dots, N) = F(1, 2, \dots, N) \Phi(1, 2, \dots, N). \quad (11)$$

Here, the total wave function Φ describes the state of N non-interacting particles. The model is adapted to the presence of interaction by introducing a correlation function, F . Using the above trial wave function with some algebra, the following cluster expansion is obtained for the energy of system,

$$E = E_1 + E_2 + E_3 + \dots \quad (12)$$

In above equation, the second term (E_2) is two-body energy, the third term (E_3) is three-body energy, and *etc.* To calculate energy of the system, we ignore higher order terms

in the cluster expansion of the energy,

$$E(S, \rho, \xi) = E_1(S, \rho, \xi) + E_2(S, \rho, \xi). \quad (13)$$

For the spin polarized liquid ^3He , besides the density and entropy, the energies are the explicit functions of spin polarization, ξ .

After some calculations, the following final expressions for E_1 and E_2 are derived,

$$E_1(S, \rho, \xi) = E_1^{(+)}(S, \rho, \xi) + E_1^{(-)}(S, \rho, \xi) \\ = \frac{\hbar^2}{4\pi^2 m \rho} \left(\int_0^\infty n^{(+)}(k, S, \rho, \xi) k^4 dk + \int_0^\infty n^{(-)}(k, S, \rho, \xi) k^4 dk \right), \quad (14)$$

$$E_2(S, \rho, \xi) = 2\pi\rho \int_0^\infty \left\{ 1 - \frac{1}{4\pi^4 \rho^2} [(\gamma^{(+)}(r, S, \rho, \xi))^2 + (\gamma^{(-)}(r, S, \rho, \xi))^2] \right\} r^2 a(r, S, \rho, \xi) dr, \quad (15)$$

where

$$\gamma^{(\pm)}(r, S, \rho, \xi) = \int_0^\infty \frac{\sin kr}{kr} n^{(\pm)}(k, S, \rho, \xi) k^2 dk, \quad (16)$$

$$a(r, S, \rho, \xi) = \frac{\hbar^2}{m} [f'(r, S, \rho, \xi)]^2 + f^2(r, S, \rho, \xi) V(r). \quad (17)$$

In Eq. (17), $f(r, S, \rho, \xi)$ is the two-body correlation function. We employ the Lennard-Jones potential as the inter-atomic potential, $V(r)$,

$$V(r) = 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right], \quad (18)$$

where $\varepsilon = 10.22 \text{ K}$ and $\sigma = 2.556 \text{ \AA}$ [34].

Now, for each value of density, entropy and spin polarization, we minimize $E_2(S, \rho, \xi)$ with respect to the variation in the correlation function. This leads to the following Euler-Lagrange differential equation,

$$f''(r, S, \rho, \xi) + f'(r, S, \rho, \xi) \frac{g'(r, S, \rho, \xi)}{g(r, S, \rho, \xi)} - \frac{m}{\hbar^2} [V(r) + \lambda] f(r, S, \rho, \xi) = 0 \quad (19)$$

where λ is the Lagrange multiplier and

$$g(r, S, \rho, \xi) = \left\{ 1 - \frac{1}{4\pi^4 \rho^2} [(\gamma^{(+)}(r, S, \rho, \xi))^2 + (\gamma^{(-)}(r, S, \rho, \xi))^2] \right\} \quad (20)$$

The two-body correlation function is obtained by numerically integrating Eq. (19), then the energy per particle of the system can be determined. Finally, for each entropy, density and spin polarization, by calculating $E(S, \rho, \xi)$, we can calculate the thermodynamic properties of the polarized liquid ^3He along different isentropic paths.

RESULTS AND DISCUSSION

As we mentioned in the previous section, using Eq. (19), the two-body correlation function $f(r)$ can be obtained as a function of the interatomic distances (r). For different values of the spin polarization (ξ), $f(r)$ has been plotted in Fig. 1 along three isentropic paths at density $\rho = 0.016 \text{ \AA}^{-3}$. what is found is that for all values of entropy and ($S = 1, 1.5$ and 2 k_B) spin polarization, the two-body correlation function reaches maximum for r in the range 2.84-2.88 \AA . Also it is found that for each spin polarization (entropy), by increasing the entropy (spin polarization), the value of correlation function at its maximum point decreases. This indicates that at high spin polarizations and entropies, the correlation between particles becomes small, inferring that the contribution of potential energy decreases by increasing the spin polarization and entropy. This behavior is getting more remarkable at high spin polarizations.

The energy per particle of the polarized liquid ^3He vs. spin polarization, ξ , for $S = 1 \text{ k}_B$ has been plotted in Fig. 2. This figure shows that there is a ferromagnetic phase transition for a specific value of density. The ferromagnetic phase transition, called spontaneous magnetization, occurs in the absence of a magnetic field. Spontaneous polarization (a nonzero value for the polarization), on the other hand, appears in the system below a certain value of control parameter (here density). Figure 2 shows that for a fixed entropy, by decreasing density, the energy per particle achieves two minima, and the ferromagnetic transition occurs around $\rho = 0.0095 \text{ \AA}^{-3}$. As far as we know, the entropy of a system is increased as the density decreases, and it is decreased as the polarization increases [17]. The balance between these two behaviors produce a fixed entropy for the

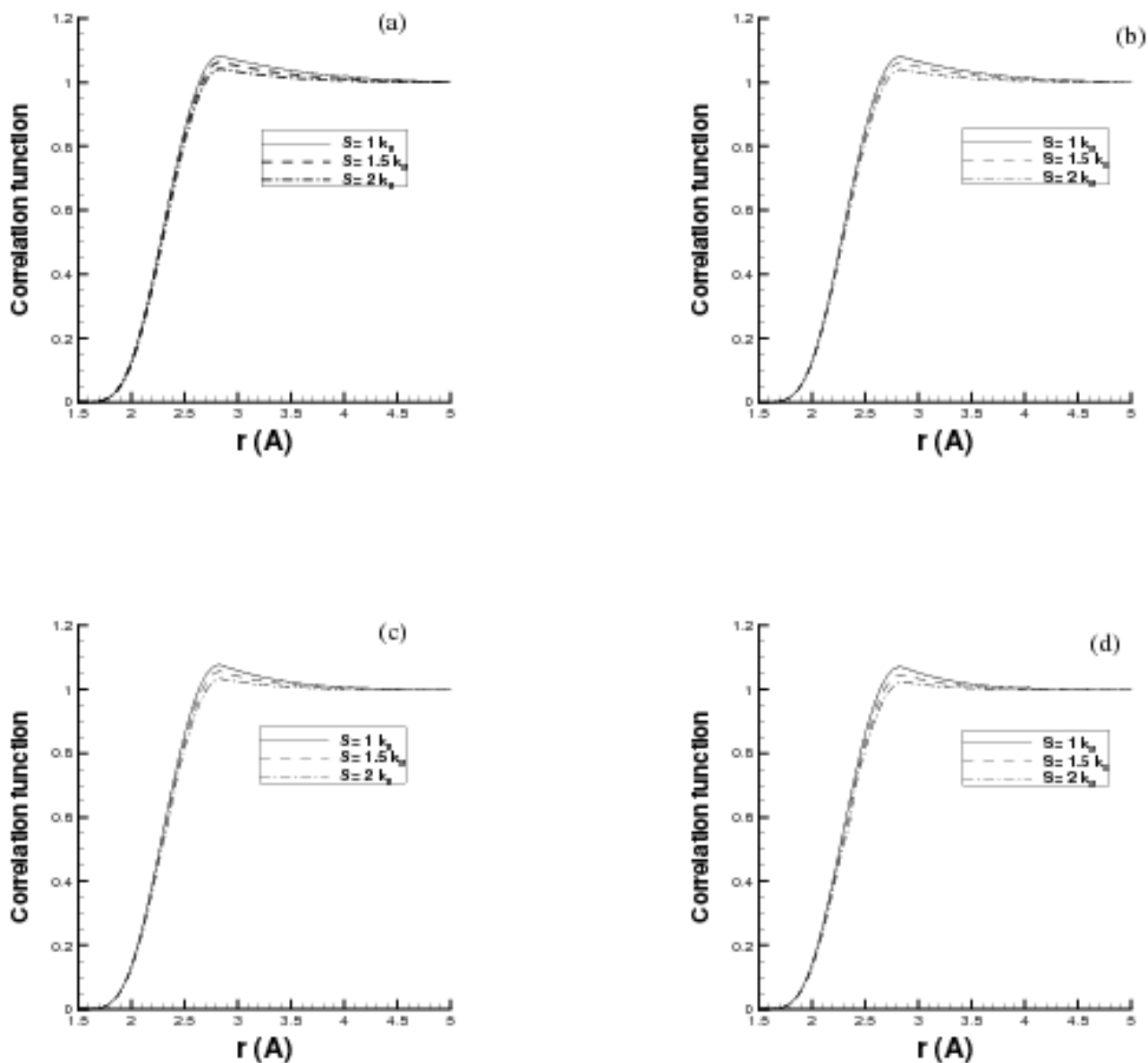


Fig. 1. The correlation function vs. the interatomic distances (r) at $\rho = 0.016 \text{ \AA}^{-3}$ for $\zeta = 0.0$ (a), 0.4 (b), 0.8 (c) and 1.0 (d).

system. This conclusion is clarified through Fig. 3, where the presence of a spontaneous polarization at densities below a certain density ($\rho = 0.0095 \text{ \AA}^{-3}$) and its absence above this density will then be interpreted as a ferromagnetic transition in the system at this density ($\rho = 0.0095 \text{ \AA}^{-3}$ for $S = 1 k_B$). Here, the polarization and density are called order parameter and control parameter, respectively.

In Fig. 4, we have shown the energy per particle of polarized liquid ^3He at $\rho = 0.008 \text{ \AA}^{-3}$ for three different values of entropy. In this figure, the entropy has been selected as a control parameter. We can see that for entropies greater than $S = 1.1 k_B$, the two minima in energy curve disappear. This indicates that for higher entropies, the minimum point of energy is only occurred at $\zeta = 0$, and the ferromagnetic transition does not happen.

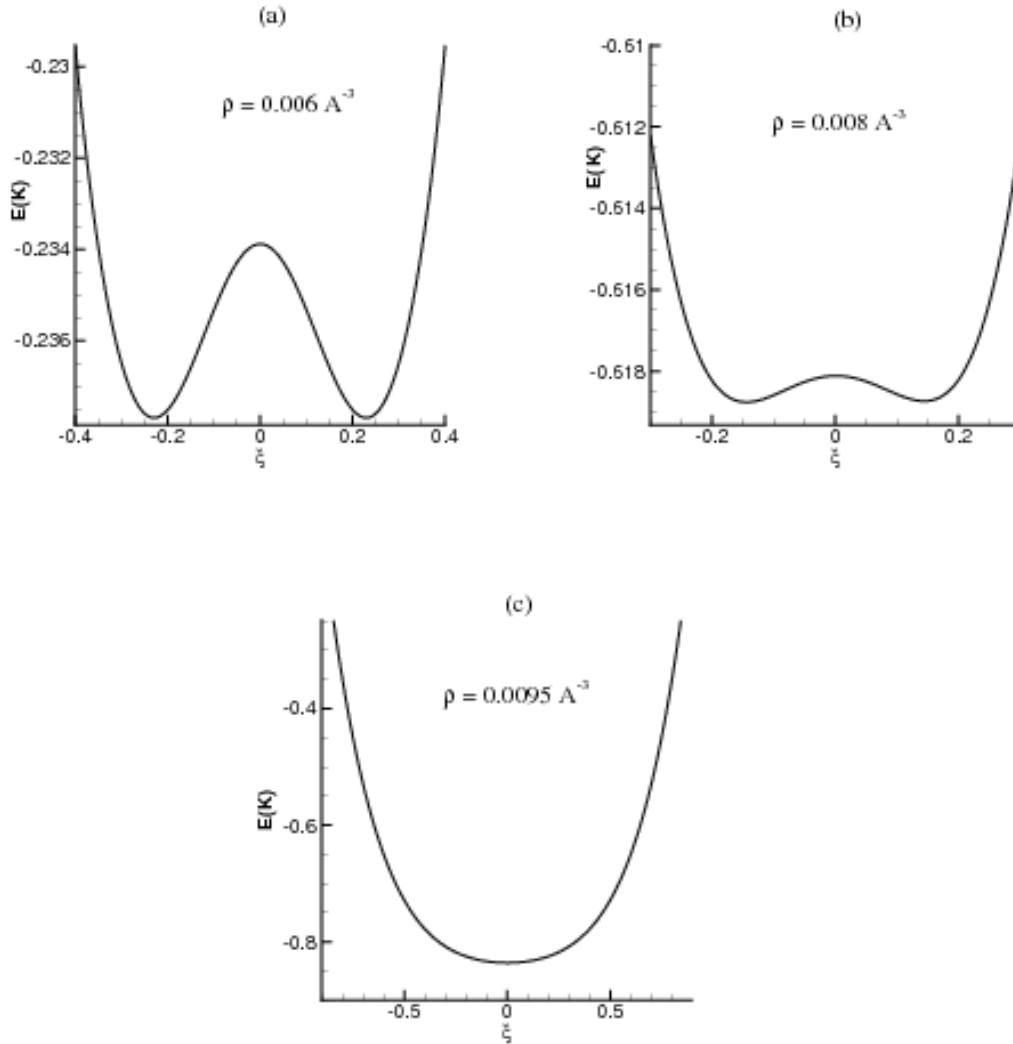


Fig. 2. The energy per particle of polarized liquid ^3He vs. the spin polarization (ξ) for $S = 1 k_B$ at $\rho = 0.006$ (a), 0.008 (b) and 0.0095 \AA^{-3} (c).

We have also drawn our results for the internal energy per particle vs. density in Fig. 5, for various spin polarizations (ξ) and entropies (S). what is seen is that energy increases by increasing the spin polarization, and this variation becomes larger at high entropies. Minimum points in the internal energy vs. density shows densities in which the system is stable. This figure shows that the minimum points of energy (stable states) for some densities (saturation densities) disappear with increasing entropy. Less stability at high entropies seems quite reasonable.

Therefore, by increasing the entropy, these minimum points must disappear. Table 1, shows the dependence of

saturation densities on both entropy and ξ . This table reveals that for each spin polarization (entropy), by increasing the entropy (spin polarization) the saturation density decreases (increases). We also see that for some values of ξ and entropy, these saturation points disappear. Based on these results, we can conclude that at high entropies, the probability of existence of such stable states (equilibrium states) is very low.

The isentropic pressure (P) is given by

$$P = \rho^2 \left. \frac{\partial E}{\partial \rho} \right|_{S, \xi} \quad (21)$$

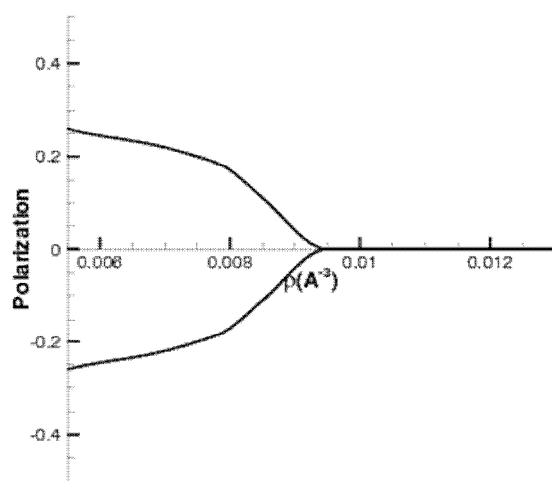


Fig. 3. The polarization corresponding to the minimum point of energy as a function of density for polarized liquid ^3He at $S = 1 k_B$.

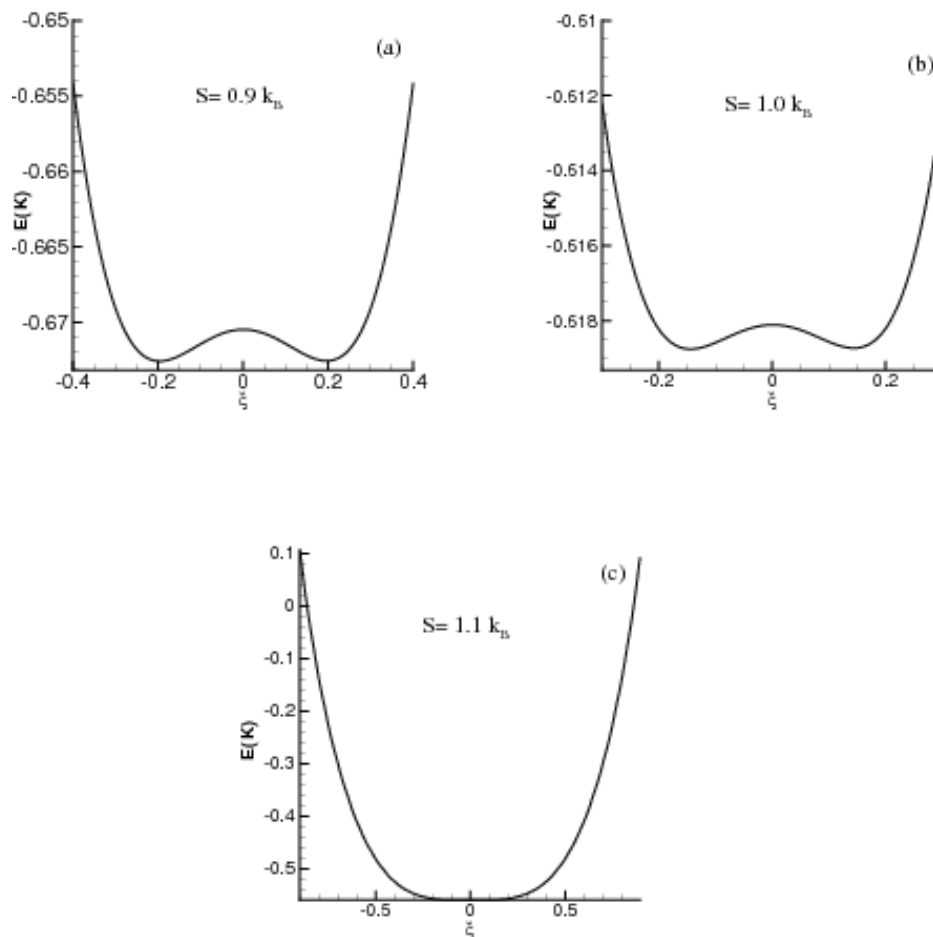


Fig. 4. The energy per particle of polarized liquid ^3He vs. the spin polarization (ξ) for $\rho = 0.008 \text{ A}^{-3}$ at $S = 0.9$ (a), 1.0 (b) and $1.1 k_B$ (c).

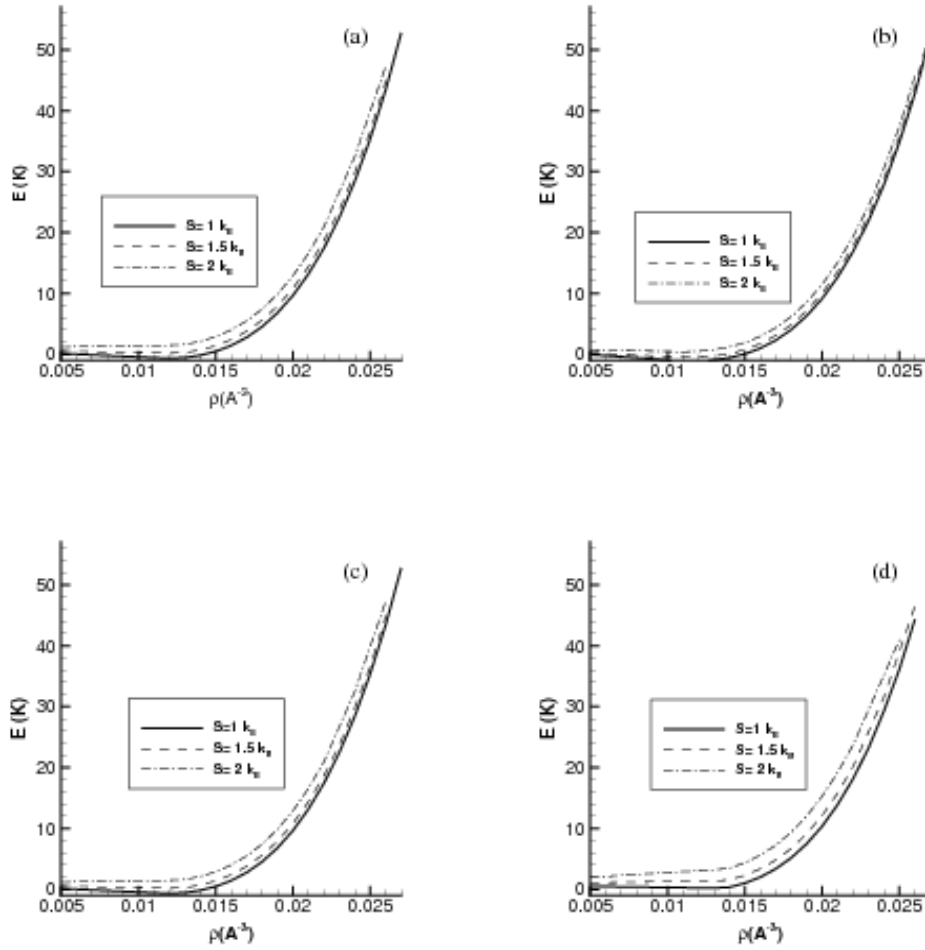


Fig. 5. The energy per particle of polarized liquid ^3He vs. density for different values of entropy (S) at $\zeta = 0.0$ (a), 0.4 (b), 0.8 (c) and 1.0 (d).

Table 1. The Saturation Density (ρ_0) at Different Values of ζ and S for the Polarized Liquid ^3He

ζ	$S(k_B)$	$\rho_0(\text{\AA}^{-3})$
0.0	1.0	0.0115
0.0	1.5	0.0115
0.0	2.0	0.0110
0.4	1.0	0.0115
0.4	1.5	0.0115
0.4	2.0	0.0110
0.8	1.0	0.0125
0.8	1.5	0.0125
0.8	2.0	-
1.0	1.0	0.0140
1.0	1.5	-
1.0	2.0	-

In Fig. 6, the pressure of polarized liquid ^3He vs. density for various entropies and ζ has been plotted. This figure clearly shows that the pressure increases by increasing both entropy and ζ . We have also found that for the fully polarized liquid ^3He ($\zeta = 1$) the difference between pressures for $S = 1.5$ and $2 k_B$ is negligible. It is shown that as the spin polarization (ζ) increases, increasing of pressure by increasing the entropy becomes faster, and the equation of state of polarized liquid ^3He becomes stiffer.

For each spin polarization and entropy, we can use the following expression to calculate the velocity of sound (v_s),

$$v_s = \left[\sqrt{\frac{\partial P}{\partial \rho}} \right]_{S, \zeta}, \quad (22)$$

where ρ is the mass density. In our previous article [30], we studied the behavior of velocity of sound in the normal liquid ^3He vs. pressure in various isentropic paths. Now, in

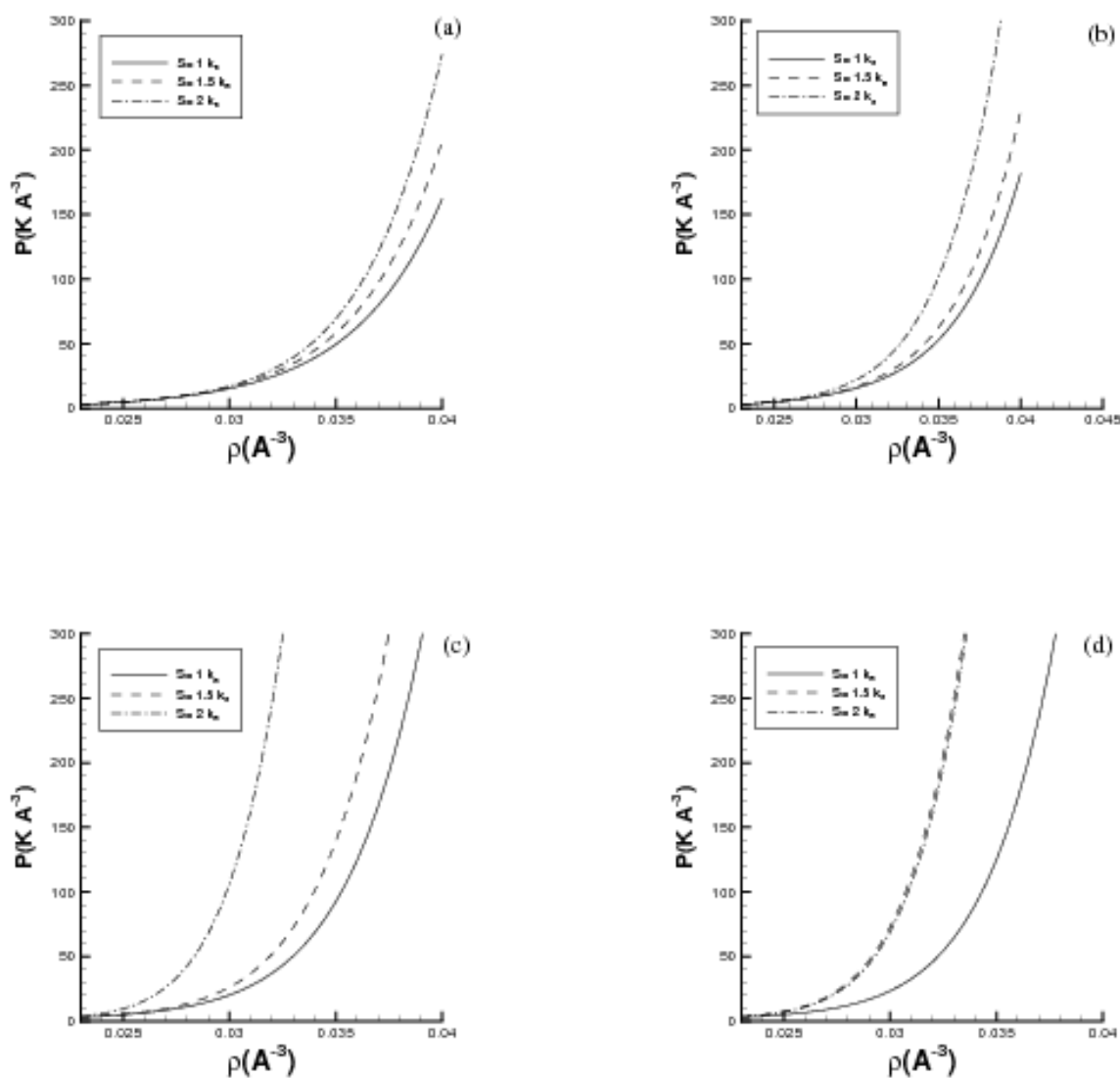


Fig. 6. As Fig. 5 but for the pressure of polarized liquid ^3He .

this work, we investigate the effect of polarization on v_s . The velocity of sound in polarized liquid ^3He vs. pressure along two different isentropic paths has been plotted in Fig. 7. In addition to the results of our previous work (decreasing the velocity of sound by increasing the entropy at a given pressure) [30], Fig. 7 shows that for small values of entropy, the effect of polarization on velocity of sound is almost negligible. But at the higher values of entropy, this effect is

considerable. We have also compared our results for the velocity of sound with those of experimental results of Ref. [25] in Fig. 7. It should be noted that this experiment has been carried out at temperature $T = 1.6\text{ K}$ for the pressures below 1 MPa . These conditions almost correspond to the higher values of entropy ($S = 2.0\text{ k}_B$) in our calculations. Figure 7 shows that at $S = 2.0\text{ k}_B$ for low pressures, our results are almost close to those reported from experimental

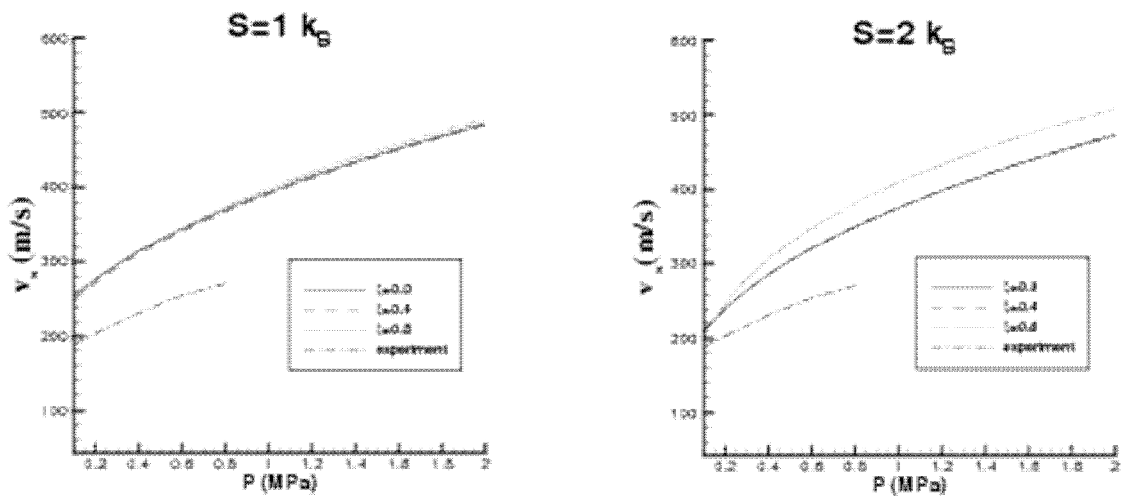


Fig. 7. Velocity of sound (v_s) in the polarized liquid ^3He vs. pressure (p) for $S = 1.0$ and 2.0 k_B at different values of spin polarization (ζ). The experimental results [25] (dashed dotted) have been also given for comparison.

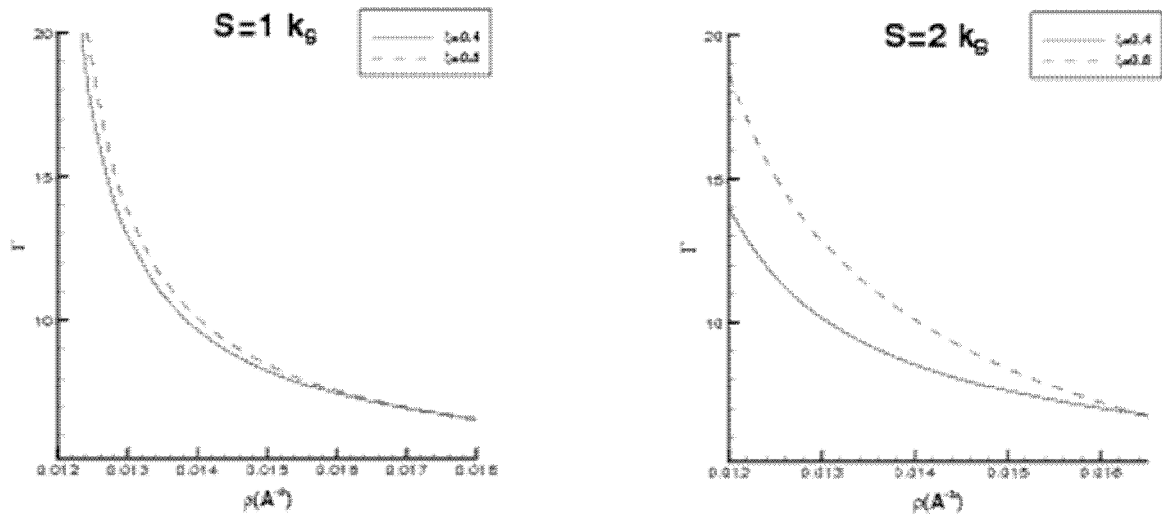


Fig. 8. Adiabatic index (γ) for the polarized liquid ^3He vs. density (ρ) at $S = 1.0$ and 2.0 k_B , and different values of spin polarization (ζ).

efforts. However, the difference between them grows by increasing the pressure. It seems that for modifying our results, we should consider other effects such as the spin-spin correlation between ^3He atoms in our calculations [35].

The isentropic expansion coefficient (adiabatic index) indicating the relation between pressure and volume during an adiabatic expansion is defined as [36],

$$\Gamma = \frac{\rho}{P} \left(\frac{\partial P}{\partial \rho} \right)_{S, \xi} \quad (23)$$

Figure 8 shows our results for adiabatic index of the polarized liquid ^3He vs. density at different spin polarization along two isentropic paths. As seen in this figure, despite the ideal gas model for this interacting system, Γ is not constant anymore, and for the relevant range of densities, it decreases by increasing density which is due to the interaction between ^3He atoms in liquid ^3He . Moreover, at each density the adiabatic index decreases by increasing the entropy. We can see that similar to the velocity of sound, the adiabatic index of polarized liquid ^3He increases by increasing the polarization, specially at higher values of entropy. According to the relation between the pressure and adiabatic index, we can conclude that by increasing the spin polarization and, therefore, increasing the adiabatic index, the equation of state becomes stiffer (Fig. 6).

For a constant value of entropy, the isentropic compressibility can be written as,

$$\beta_S = -\frac{1}{V} \left(\frac{\partial V}{\partial P} \right)_{S, \xi} \quad (24)$$

where $V = \frac{V}{N} = \frac{1}{\rho}$ [1]. Variations of compressibility of polarized liquid ^3He vs. polarization, at different values of density for a fixed entropy ($S = 1 k_B$) has been shown in Fig. 9. It is interesting to note that throughout the whole range of polarization in our calculation, the absolute value of compressibility remains nearly constant, especially at high densities. Our results show that the isentropic compressibility is almost insensitive to the polarization changes, especially at high densities. It is also found that for each value of polarization, compressibility is decreased as the density increases. We have realized that there is an

overall agreement between our results for compressibility and the results of other theoretical methods for zero temperature [27].

In Fig. 10, the temperature of polarized liquid ^3He has been shown as a function of density for three different entropies at various spin polarizations. It is seen that the temperature is increased as the entropy, spin polarization and density increase. Indeed by increasing the density, contribution of kinetic energy increases which leads to increasing the temperature. Finally, we have found that for each entropy, the difference between the temperatures of fully polarized and unpolarized liquid ^3He increases for higher values of density, especially at high entropies.

SUMMARY AND CONCLUSION

In the present work, we have used the variational method to calculate some thermodynamic properties of the polarized liquid ^3He along different isentropic paths. The potential employed in this paper is Lennard-Jones potential. For all values of spin polarization, our calculations show a maximum for the two-body correlation function in the interatomic distances about $r = 2.8 \text{ \AA}$. It was found that the correlation between ^3He atoms reduces as the entropy and spin polarization increase. This leads to decreasing the contribution of potential energy by increasing the entropy and spin polarization. We have reported the appearance of a spontaneous polarization in the system, where the energy per particle achieves two minima for some nonzero values of ξ , and the ferromagnetic transition occurs for the certain values of density and entropy. Also, our results for the internal energy per particle versus density indicate that the energy increases by increasing the spin polarization, and by increasing the entropy, the minimum points of energy disappear. Furthermore, we have found that for a specific value of spin polarization (entropy), the saturation density is decreased (increased) by increasing the entropy (spin polarization). Insignificant effect of spin polarization on velocity of sound for the lower entropies has been found in this work. It is seen that by increasing the polarization, the adiabatic index of polarized liquid ^3He increases, and the equation of state becomes stiffer, specially at higher entropies. Our calculations have shown that at a specific value of entropy, for all values of relevant density, the

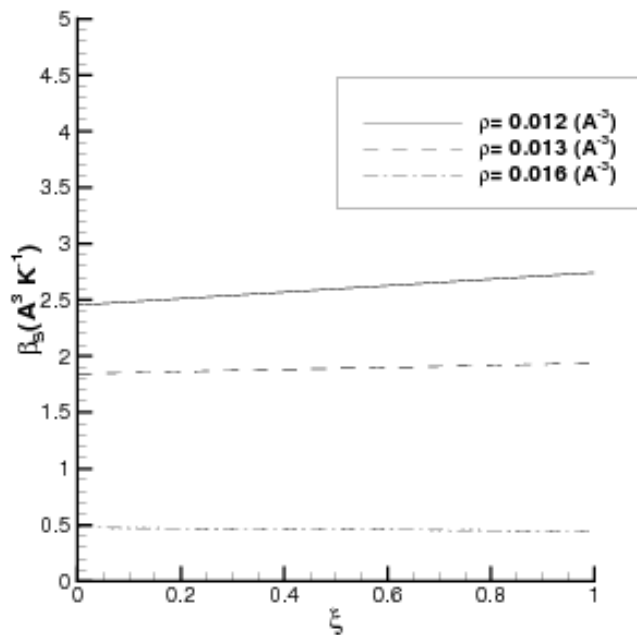


Fig. 9. Isentropic compressibility of polarized liquid ^3He vs. spin polarization (ξ) for $S = 1 k_B$ at different values of density (ρ).

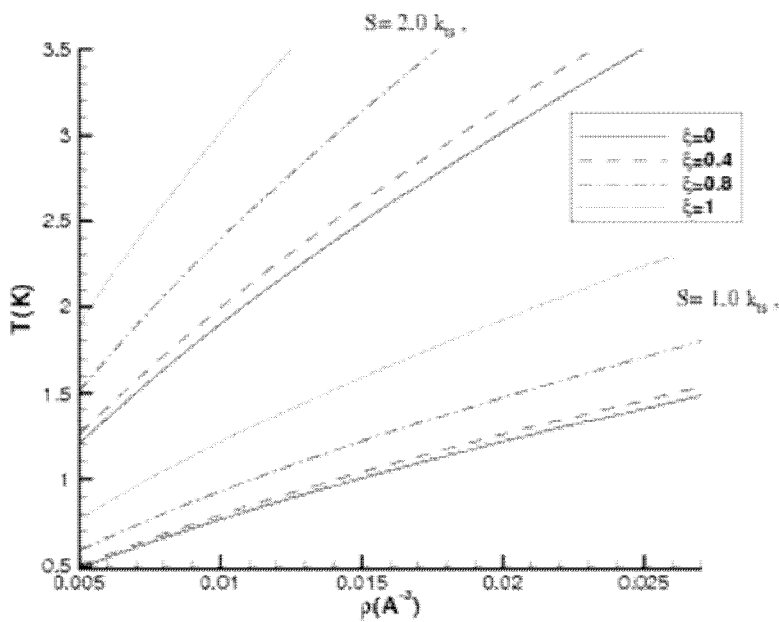


Fig. 10. The temperature of polarized liquid ^3He vs. density for different values of spin polarization (ξ) and entropies (S).

compressibility remains nearly constant by increasing the polarization. It has been also verified that by increasing spin polarization and entropy, the pressure and temperature of polarized liquid ^3He increase. Finally, a comparison has been made with the results of experiment indicating that it is needed to consider other effects such as the spin-spin correlation between ^3He atoms to modify our calculations.

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