Lowest Order Constrained Variational calculation for Polarized Liquid $^3$He at Finite Temperature

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Abstract

We have investigated some of the thermodynamic properties of spin polarized liquid $^3$He at finite temperature using the lowest order constrained variational method. For this system, the free energy, entropy and pressure are calculated for different values of the density, temperature and polarization. We have also presented the dependence of specific heat, saturation density and incompressibility on the temperature and polarization.

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I. INTRODUCTION

The spin polarized liquid $^3$He at finite temperature is an interesting many-body system which obeys the Fermi-Dirac statistics. Several theoretical techniques and experimental method have been used for investigating the properties of unpolarized liquid $^3$He \[1, 2, 3, 4, 5, 6, 7, 8\]. Recently, we have studied the unpolarized liquid $^3$He at finite temperature and the spin polarized liquid $^3$He at zero temperature \[9, 10, 11\]. In this calculations, we have applied the lowest order constrained variational method based on the cluster expansion of the energy functional. This method is a powerful microscopic technique used in the many-body calculations of dense matter \[9, 10, 11, 12, 13, 14, 15, 16, 17, 18\].

In the present work, we use the lowest order constrained variational method to investigate some of the thermodynamic properties of spin polarized liquid $^3$He at finite temperature. In our calculations, we employ the Lennard-Jones \[19\] and Aziz \[20\] potentials.

II. METHOD

We consider a system consisting of $N$ interacting $^3$He atoms with $N^+$ spin up and $N^-$ spin down atoms. These atoms have a different chemical potential ($\mu$) and different Fermi-Dirac distribution function \[23\] as follows,

$$n^\pm(k) = \frac{1}{\exp[\beta(\frac{k^2}{2m} - \mu^\pm)] + 1},$$  \hspace{1cm} (1)

where $\beta = \frac{1}{k_BT}$ and $T$ is the temperature. We define the total number density by $\rho$ and the spin asymmetry parameter by $\xi$ ($\xi = 0$ is unpolarized and $\xi = 1$ is fully polarized cases),

$$\rho = \rho^+ + \rho^-, \hspace{1cm} \xi = \frac{N^+ - N^-}{N^+ + N^-}. \hspace{1cm} (2)$$

Thus, to determine the chemical potential for every $\rho$, $T$ and $\xi$, we solve the following equation by numerical method,

$$\rho^\pm = \frac{1}{2\pi^2} \int_0^\infty n^\pm(k)k^2dk.$$

(3)

We calculate the energy using the lowest order constrained variational method based on the cluster expansion of the energy. We consider up to the two-body energy term in cluster
expansion,

\[ E = E_1 + E_2. \]  

(4)

For this system, the one-body energy per particle, \( E_1 \), is given by

\[
E_1 = E_1^+ + E_1^-
= \frac{\hbar^2}{4m\pi^4\rho} \left[ \int_0^\infty n^+(k)k^4dk + \int_0^\infty n^-(k)k^4dk \right].
\]  

(5)

The two-body energy per particle, \( E_2 \), is defined

\[
E_2 = \frac{1}{2N} \sum_{i,j} \langle ij | W(12) | ij - ji \rangle,
\]  

(6)

where

\[
W(r_{12}) = \frac{\hbar^2}{m} (\nabla f(r_{12}))^2 + f^2(r_{12})V(r_{12}).
\]  

(7)

In the above equation, \( V(r_{12}) \) is the two body potential between helium atoms and \( f(r_{12}) \) is the two-body correlation function. By considering the \( |i\rangle \) as a plane wave, we have derived the following relation for the two-body energy per particle,

\[
E_2 = \frac{1}{2\rho} \int d\mathbf{r} \left[ 1 - \frac{1}{4\pi^4\rho^2} \left( (\gamma^+(r))^2 + (\gamma^-(r))^2 \right) \right] W(r),
\]  

(8)

where

\[
\gamma^\pm(r) = \int_0^\infty \frac{\sin(kr)}{kr} n^\pm(k)k^2dk.
\]  

(9)

Now, we minimize the two-body energy Eq. (8) with respect to the variations in the two-body correlation function subject to the normalization constraint [21, 22],

\[
\frac{1}{N} \sum_{i,j} \langle ij \mid h^2(r_{12}) - f^2(r_{12}) \mid ij - ji \rangle = 1.
\]  

(10)

The normalization constraint is conveniently re-written in the integral form as

\[
\rho \int d\mathbf{r} [h^2(r) - f^2(r)] \Gamma(r) = 1,
\]  

(11)

where

\[
\Gamma(r) = \left[ 1 - \frac{1}{4\pi^4\rho^2} \left( (\gamma^+(r))^2 + (\gamma^-(r))^2 \right) \right].
\]  

(12)

and \( h(r) \) is the Pauli function,

\[
h(r) = [\Gamma(r)]^{-\frac{1}{2}}.
\]  

(13)
The minimization of the two-body Energy $E_2$ gives the following Euler-Lagrange differential equation for the two-body correlation function

$$f''(r) + f'(r) \frac{\Gamma'(r)}{\Gamma(r)} - \frac{m}{\hbar^2} (\lambda + V(r)) f(r) = 0.$$  

(14)

The lagrange multiplier $\lambda$ imposes by normalization constraint. The two-body correlation function calculated by numerically integrating Eq. (14) and then the energy per particle of system can be obtained. Finally the Helmholtz free energy per particle can be determined using the following equation,

$$F = E - TS.$$  

(15)

$S$ is the entropy per particle \[23\] which is given by

$$S = S^+ + S^-,$$  

(16)

where

$$S^\pm = - \frac{1}{2\pi^2 \rho} \int_0^\infty \left[ n^\pm(k) \ln(n^\pm(k)) + (1 - n^\pm(k)) \ln(1 - n^\pm(k)) \right] k^2 dk.$$  

(17)

By calculating $E$, $S$ and $F$, we can obtain the thermodynamic properties of the spin polarized liquid $^3$He at finite temperature.

### III. RESULTS

The two-body correlation function at $T = 1.0K$ and $T = 4.0K$ for different values of the spin asymmetry parameter ($\xi$) are shown in Fig. 1. This figure shows that at low temperatures, the correlation function increases more rapidly and reaches the limiting value ($f(r) = 1$) at larger interatomic distances ($r$). It is shown that by increasing $\xi$, the correlation function reaches the limiting value at lower $r$. It is seen that our results for the correlation function with the Lennard-Jones and Aziz potentials are identical.

Our results for the free energy of liquid $^3$He with the Lennard-Jones and Aziz potentials at different spin asymmetry parameters ($\xi$) are presented in Fig. 2. We can see that at low densities ($\rho < 0.011A^{-3}$), the free energies with the Lennard-Jones and Aziz potentials are similar. However, at higher densities, the difference between these free energies are noticeable. Fig. 2 shows that the free energy increases by increasing spin asymmetry parameter and this variation becomes higher at high temperatures. We see that the free energy doesn’t show a bound state above a certain value of temperature (called flashing...
temperature, $T_f$). We have found $T_f$ for different values of $\xi$ which given in Table I. From Fig. 2, it is also seen that for each value of spin asymmetry parameter, the density of saturation point (minimum point of the free energy) decreases by increasing temperature. We see that the saturation density ($\rho_0$) increases by increasing spin asymmetry parameter for each value of temperature. Our results for the saturation density are given in Table II.

Table I (Table II) shows that for all values of $\xi$ the flashing temperature (the saturation density) with the Aziz potential is lower than that of the Lennard-Jones potential.

The entropy of liquid $^3$He is shown as a function of density for two different temperatures and various asymmetry parameters in Fig. 3. It is seen that the entropy decreases by increasing both density and spin asymmetry parameter and increases by increasing temperature. We have found that for each temperature, the difference between entropy of fully polarized and unpolarized liquid $^3$He decreases for higher values of density, especially at low temperatures.

In Figs. 4-6, we have shown the free energy, entropy and the specific heat of liquid $^3$He as a function of temperature for different values of $\xi$ at $\rho = 0.0166 A^{-3}$. In these figures, the experimental results [1] for the unpolarized liquid $^3$He are also shown for comparison. Fig. 4 indicates a good agreement between our results for the free energy with the Lennard-Jones potential and the experimental results. From Figs. 4-6, it is seen that the free energy (entropy and specific heat) decreases (increase) by increasing temperature. In addition, we see that for the free energy, entropy and the specific heat of liquid $^3$He, the differences between fully polarized and unpolarized cases increase by increasing temperature.

The isothermal pressure is obtained from the free energy using the following equation,

$$P(\rho, T) = \rho^2 \frac{\partial F(\rho, T)}{\partial \rho}.$$  \hspace{1cm} (18)

In Fig. 7, we have plotted the isothermal pressure as a function of density for the various temperatures and $\xi$. It is seen that the equation of state with the Aziz potential is stiffer than that of the Lennard-Jones potential. This figure shows that at low temperatures we have a liquid-gas phase equilibrium for the liquid $^3$He. We know that at the critical temperature ($T_c$) there is no liquid-gas phase equilibrium. Our results of the critical temperature for different values of $\xi$ are presented in Table III. We see that the critical temperature increases by increasing $\xi$. For all $\xi$ it is seen that the ($T_c$) with the Aziz potential is lower than that of the Leonard-Jones potential.
For liquid $^3$He, the saturation incompressibility at saturation density is given by,

$$K_0(T) = 9 \left( \rho^2 \frac{\partial^2 F(\rho, T)}{\partial \rho^2} \right)_{\rho_0}.$$  \hfill (19)

In Table III, our calculated values of the saturation incompressibility are presented for different values of $\xi$ and $T$. It is seen that for each value of $\xi$, the incompressibility decreases by increasing temperature and at each temperature, it increases by increasing $\xi$. From Table III we see that for all values of spin asymmetry parameter our results for the $K_0$ with the Aziz potential are lower than those of the Leonard-Jones potential.

IV. SUMMARY AND CONCLUSION

We have considered a system consisting of the Helium atoms ($^3$He) with an asymmetrical spin configuration. For this system, we have calculated some of the thermodynamic properties using the lowest order constrained variational method with the Lennard-Jones and Aziz potentials. Our calculations lead to the following conclusions for the liquid $^3$He:

- At high temperatures, the correlation function reaches the limiting value for the smaller values of the interatomic distances.

- The results of the correlation function with the Lennard-Jones and Aziz potentials are very similar.

- The free energy with the the Lennard-Jones and Aziz potentials are identical for small values of the density.

- The free energy, saturation density and incompressibility decrease by increasing temperature.

- The free energy, saturation density, incompressibility and critical temperature increase by increasing spin asymmetry parameter.

- The entropy, specific heat and flashing temperature decrease by increasing spin asymmetry parameter.

- The entropy decreases by increasing density and increases by increasing temperature.
• The equation of state with the Aziz potential is stiffer than that of the Lennard-Jones potential.

• For all values of spin asymmetry parameter our results for the flashing temperature, saturation density, critical temperature and saturation incompressibility with the Aziz potential are lower than those of the Leonard-Jones potential.

Acknowledgments

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TABLE I: The flashing temperature ($T_f$) for different values of $\xi$.

| $\xi$ | $T_f(K)$ | $T_f(K)$ |
|-------|----------|----------|
| 0.0   | 2.8      | 2.6      |
| 0.4   | 2.7      | 2.5      |
| 0.8   | 2.6      | 2.3      |
| 1.0   | 2.2      | 1.9      |

TABLE II: The saturation density ($\rho_0$) and the saturation incompressibility ($K_0$) of liquid $^3$He for different values of $\xi$ and temperature.

| $\xi$ | $T(K)$ | $\rho_0(A^{-3})$ | $K_0(K)$ | $\rho_0(A^{-3})$ | $K_0(K)$ |
|-------|--------|-------------------|----------|-------------------|----------|
| 0.0   | 0.5    | 0.0117            | 185      | 0.011             | 174      |
| 0.0   | 1.0    | 0.0116            | 163      | 0.0109            | 157      |
| 0.0   | 1.5    | 0.0113            | 135      | 0.0106            | 121      |
| 0.4   | 0.5    | 0.0117            | 187      | 0.011             | 183      |
| 0.4   | 1.0    | 0.0116            | 172      | 0.0109            | 162      |
| 0.4   | 1.5    | 0.0114            | 145      | 0.0107            | 132      |
| 0.8   | 0.5    | 0.0120            | 237      | 0.0113            | 212      |
| 0.8   | 1.0    | 0.0120            | 232      | 0.0113            | 206      |
| 0.8   | 1.5    | 0.0119            | 203      | 0.0112            | 179      |
| 1.0   | 0.5    | 0.0128            | 275      | 0.0119            | 260      |
| 1.0   | 1.0    | 0.0128            | 263      | 0.0119            | 246      |
| 1.0   | 1.5    | 0.0127            | 212      | 0.0118            | 204      |
TABLE III: The critical temperature ($T_c$) for different values of $\xi$.

| $\xi$ | $T_c(K)$ | $T_c(K)$ |
|-------|----------|----------|
| 0.0   | 5.3      | 5.1      |
| 0.4   | 5.5      | 5.3      |
| 0.8   | 6.2      | 5.8      |
| 1.0   | 6.5      | 6.1      |
FIG. 1: The correlation function versus the interatomic distance (r) with the Leonard-Jones (full curves) and Aziz (dotted curves) potentials at ρ = 0.0166Å⁻³ for ξ = 0.0 (a), ξ = 0.4 (b), ξ = 0.8 (c) and ξ = 1.0 (d).
FIG. 2: The free energy of liquid $^3$He versus density at different values of temperature ($T = 1.0, 2.0, 3.0, 4.0, 5.0 K$) with the Leonard-Jones (full curves) and Aziz (dotted curves) potentials for $\xi = 0.0$ (a), $\xi = 0.4$ (b), $\xi = 0.8$ (c) and $\xi = 1.0$ (d).
FIG. 3: The entropy of liquid $^3$He versus density at $T = 1.0K$ and $T = 4.0K$ for different values of $\xi$.  

\[ \xi = 0.0 \] 
\[ \xi = 0.4 \] 
\[ \xi = 0.8 \] 
\[ \xi = 1.0 \]
FIG. 4: The free energy of liquid $^3$He versus temperature for $\rho = 0.0166\,\text{Å}^{-3}$ at different values of $\xi$ with the Leonard-Jones (full curves) and Aziz (dotted curves) potentials. The experimental results (dashed curve) for unpolarized liquid $^3$He [1] are also shown for comparison.
FIG. 5: The entropy of liquid $^3$He versus temperature for $\rho = 0.0166A^{-3}$ at different values of $\xi$. 
FIG. 6: As Fig. [1] but for the specific heat.
FIG. 7: The pressure versus density at different values of temperature ($T = 1.0, 3.0, 5.0, 6.0 K$) with the Leonard-Jones (full curves) and Aziz (dotted curves) potentials for $\xi = 0.0$ (a), $\xi = 0.4$ (b), $\xi = 0.8$ (c) and $\xi = 1.0$ (d).