Spin polarized liquid $^3$He

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Abstract

We have employed the constrained variational method to study the influence of spin polarization on the ground state properties of liquid $^3$He. The spin polarized phase, we have found, has stronger correlation with respect to the unpolarized phase. It is shown that the internal energy of liquid $^3$He increases by increasing polarization with no crossing point between polarized and unpolarized energy curves over the liquid density range. The obtained internal energy curves show a bound state, even in the case of fully spin polarized matter. We have also investigated the validity of using a parabolic formula for calculating the energy of spin polarized liquid $^3$He. Finally, we have compared our results with other calculations.

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I. INTRODUCTION

The spin polarized liquid $^3$He is an interesting quantum many-body system which can be experimentally examined. In fact, it is expected that this phase of liquid $^3$He has a large life time to be observed in a quasi-thermodynamic equilibrium [1, 2, 3, 4, 5, 6].

Some theoretical investigations have been done for spin polarized liquid $^3$He using different approaches such as Green’s function Monte Carlo (GFMC), Fermi hyper-netted chain (FHNC), correlated basis functions (CBF) and transport theory [7, 8, 9, 10, 11, 12, 13]. Recently, we have studied the unpolarized liquid $^3$He and calculated some of its thermodynamic properties at finite temperature. A good agreement between our results and corresponding empirical values has been shown [14, 15]. In these calculations, constrained variational method based on the cluster expansion of the energy functional has been used. This method is a powerful microscopic technique used in many-body calculations of dense matter [16, 17, 18, 19, 20, 21, 22]. In this article, we employ this method to investigate the ground state of spin polarized liquid $^3$He.

II. CONSTRAINED VARIATIONAL CALCULATION OF SPIN POLARIZED LIQUID $^3$He

To calculate the ground state energy of spin polarized liquid $^3$He, consisting of $N$ interacting atoms with $N^+$ spin up and $N^-$ spin down atoms, $N = N^+ + N^-$, we use the variational calculation based on the cluster expansion of the energy functional [23]. We consider up to the two-body energy term in the cluster expansion,

$$E = E_1 + E_2.$$  \hspace{1cm} (1)

The one-body energy per particle for the spin polarized matter is given by

$$E_1 = E_1^{(+)} + E_1^{(-)} = \frac{3}{10} \left( \frac{\hbar^2}{2m} \right) (3\pi^2)^{2/3} \left[ (1 + \xi)^{5/3} + (1 - \xi)^{5/3} \right] \rho^{2/3},$$ \hspace{1cm} (2)

where $\rho$ is the total number density,

$$\rho = \rho^{(+)} + \rho^{(-)}.$$ \hspace{1cm} (3)
and the spin asymmetry parameter, $\xi$, is defined to be

$$\xi = \frac{N^+(+) - N^(-)(-)}{N}.$$  \hspace{1cm} (4)$$

$\xi$ shows the spin ordering of the matter which can get a value in the range of $\xi = 0.0$ (unpolarized matter) to $\xi = 1.0$ (fully polarized matter).

To obtain the two-body energy term, $E_2$, we can start from the known equation

$$E_2 = \frac{1}{2} \sum_{ij} <ij|W(12)|ij>_a,$$

where

$$W(12) = \frac{\hbar^2}{m} \left( \nabla f(12) \right)^2 + f^2(12)V(12),$$

and $V(12)$ is the two-body potential between the helium atoms (we use the Lennard-Jones potential with $\epsilon = 10.22 \text{ K}$ and $\sigma = 2.556 \text{ A}$) and $f(12)$ is two-body correlation function.

By considering the $|i>$ as a plane wave and performing some algebra, we have derived the following relation for the spin polarized matter,

$$E_2 = \frac{1}{2} \rho^2 \int dr_1 \int dr_2 \left[ 1 - \frac{1}{4} \left[ (1 + \xi)^2 \ell^2(k_F^+(r_{12}) + (1 - \xi)^2 \ell^2(k_F^-(r_{12})) \right] \right] W(r_{12}),$$

where

$$\ell(x^{(i)}) = \frac{3}{(x^{(i)})^3} \left[ \sin(x^{(i)}) - x^{(i)} \cos(x^{(i)}) \right],$$

and $x^{(i)}$ is $k_F^+(r_{12})$ or $k_F^-(r_{12})$. $k_F^+(r_{12}) = (6\pi^2 \rho(r_{12}))^{1/3}$ and $k_F^-(r_{12}) = (6\pi^2 \rho(r_{12}))^{1/3}$ are the Fermi momentum of spin up and spin down states, respectively. By minimizing the Eq. (7) with respect to the $f(12)$, the following differential equation is obtained:

$$\frac{d}{dr} \left[ L(r) f'(r) \right] - \frac{m}{\hbar^2} \left[ V(r) + \lambda \right] L(r)f(r) = 0,$$

where

$$L(r) = 1 - \frac{1}{4} \left[ (1 + \xi)^2 \ell^2(k_F^+(r_{12}) + (1 - \xi)^2 \ell^2(k_F^-(r_{12})) \right],$$

and $\lambda$ is the lagrange multiplier which imposes the constraint of the two-body wave function normalization. Eq. (9) can be solved numerically and the correlation function $f(12)$ and finally the internal energy of system are obtained.
III. RESULTS

The numerical results for the two-body correlation function of liquid $^3$He are given in Fig. 1. This shows that for the higher value of spin asymmetry parameter, the correlation function increases more rapidly and reaches to the limiting value ($f(r) = 1$) at smaller value of $r$. From Fig. 1 we can see that in the case of higher polarization, the helium atoms have a stronger correlation at short relative distance.

The numerical values of kinetic, potential and internal energy of liquid $^3$He for the different polarizations versus total number density are presented in Tables I-IV. Our results of internal energy for different spin asymmetry parameters are compared in Fig. 2. This figure indicates that as polarization increases, the internal energy gets the higher values over the liquid density range and there is no crossing point between the internal energy curves of polarized and unpolarized cases in this region. This behavior is in agreement with experiment [10, 12, 13]. A comparison between Tables I, II, III and IV shows that for each density, the kinetic energy (potential energy) increases (decreases) by increasing spin asymmetry parameter. Over the liquid density range, the increasing of kinetic energy dominates which leads to the higher internal energies. From Fig. 2, it can be also seen that for all values of $\xi$, the energy curve has a minimum which shows the existence of a bound state for this system, even for the fully polarized matter ($\xi = 1.0$). We see that by increasing the spin asymmetry parameter, this minimum point of energy curve shifts to the higher densities.

To compare our method with the well-known many-body techniques, we present the results of Green’s function Monte Carlo (GFMC) and Fermi hyper-netted chain (FHNC) calculations in Figs. 3-6. In Fig. 3, the internal energy of fully polarized and unpolarized liquid $^3$He calculated with GFMC method [12, 13] have been compared with our results. There are two points that we can mention from this figure. First, the crossing point problem exist and secondly, for all densities approximately greater than 0.014$A^{-3}$, the energy of polarized case is lower than unpolarized case which are not acceptable from the experiment. However, these problems do not exist in our method, although we should include the three-body correlation effect to obtain a better result. In Figs. 4-6 the results of FHNC method for different choices of wave function [10] are presented. We can see from these figures that before considering the backflow effect (momentum dependent two-body correlation), the polarized curve is always lower than the unpolarized curve. However after performing
extra calculations, the appropriate results have been obtained in Fig. 6. This shows that our constrained variational method can do the job much simpler, although we still need to add the three-body cluster energy to obtain a better result \cite{22,24}.

There is a similarity between spin asymmetry parameter in our calculations and isospin asymmetry parameter in nuclear matter calculations in which the energy of asymmetrical nuclear matter can be calculated using the parabolic approximation. In this approximation, one considers only the quadratic term in asymmetry parameter as well as the energy of symmetric matter \cite{21}. In a similar way, we can define the following relation for the internal energy of spin polarized liquid $^3$He:

\begin{equation}
E(\rho, \xi) = E(\rho, \xi = 0) + a_{\text{asym.}}(\rho) \xi^2,
\end{equation}

where the above equation gives the definition of spin asymmetry energy $a_{\text{asym.}}$ as:

\begin{equation}
a_{\text{asym.}}(\rho) = E(\rho, \xi = 1) - E(\rho, \xi = 0).
\end{equation}

$E(\rho, \xi = 0)$ is the internal energy of unpolarized matter which has a symmetric configuration in spin state and $E(\rho, \xi = 1)$ is the internal energy of fully polarized matter. It is now interesting to see if this approximation, Eq. (11), agrees with our microscopic calculations. For this purpose, we have compared the internal energy of spin polarized liquid $^3$He at different $\xi$ for both microscopic calculation and using parabolic approximation in Tables V and VI. These tables indicate an agreement between these two approaches, specially at high densities.

\section*{IV. SUMMARY AND CONCLUSION}

We have considered a system consisting of $N$ Helium atoms ($^3$He) with an asymmetrical spin configuration and derived the two-body term in the the cluster expansion of the energy functional. Then, we have minimized the two-body energy term under the normalization constraint and obtained the differential equation. The numerical results of internal energy of this system have been presented for different values of spin asymmetry parameter and density. It is found that as the polarization of liquid $^3$He increases, the two-body correlation becomes stronger. Over the liquid density range, our results show that the internal energy of liquid $^3$He increases by increasing spin asymmetry parameter with no crossing point between polarized and unpolarized energy curves. This shows an agreement with experimental
results. It is also seen that there is a bound state for all values of polarization. The validity of using parabolic approximation in calculating the energy of spin polarized matter is shown. Therefore, by using this approximation one can preform calculations for the spin polarized matter much simpler. we have also compared our results with other calculations to show that why of our constrained variational method is a powerful technique.

Acknowledgments

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TABLE I: Kinetic energy (KE), potential energy (PE) and internal energy of unpolarized liquid $^3$He ($\xi = 0.0$) versus total number density.

| Density ($A^{-3}$) | KE (K) | PE (K) | Internal Energy (K) |
|---------------------|--------|--------|---------------------|
| 0.003               | 0.960  | -0.832 | 0.128               |
| 0.005               | 1.349  | -1.578 | -0.228              |
| 0.007               | 1.689  | -2.341 | -0.651              |
| 0.009               | 1.997  | -3.176 | -1.178              |
| 0.011               | 2.283  | -3.864 | -1.581              |
| 0.013               | 2.552  | -4.049 | -1.496              |
| 0.015               | 2.807  | -3.386 | -0.578              |
| 0.017               | 3.052  | -1.422 | 1.629               |
| 0.019               | 3.287  | 2.321  | 5.608               |

TABLE II: As Table I but for spin polarized liquid $^3$He at $\xi = 1/3$.

| Density ($A^{-3}$) | KE (K) | PE (K) | Internal energy (K) |
|---------------------|--------|--------|---------------------|
| 0.003               | 1.019  | -0.922 | 0.096               |
| 0.005               | 1.433  | -1.701 | -0.268              |
| 0.007               | 1.794  | -2.482 | -0.688              |
| 0.009               | 2.121  | -3.256 | -1.135              |
| 0.011               | 2.424  | -3.957 | -1.532              |
| 0.013               | 2.710  | -4.154 | -1.444              |
| 0.015               | 2.981  | -3.505 | -0.523              |
| 0.017               | 3.241  | -1.555 | 1.685               |
| 0.019               | 3.491  | 2.176  | 5.667               |
TABLE III: As Table II but for spin polarized liquid $^3$He at $\xi = 2/3$.

| Density ($A^{-3}$) | KE (K) | PE (K) | Internal energy (K) |
|--------------------|--------|--------|---------------------|
| 0.003              | 1.202  | -1.133 | 0.069               |
| 0.005              | 1.689  | -1.968 | -0.279              |
| 0.007              | 2.114  | -2.766 | -0.652              |
| 0.009              | 2.499  | -3.518 | -1.018              |
| 0.011              | 2.857  | -4.240 | -1.382              |
| 0.013              | 3.194  | -4.477 | -1.283              |
| 0.015              | 3.514  | -3.863 | -0.349              |
| 0.017              | 3.819  | -1.945 | 1.874               |
| 0.019              | 4.114  | 1.754  | 5.868               |

TABLE IV: As Table II but for fully polarized liquid $^3$He ($\xi = 1.0$).

| Density ($A^{-3}$) | KE (K) | PE (K) | Internal energy (K) |
|--------------------|--------|--------|---------------------|
| 0.003              | 1.524  | -1.403 | 0.120               |
| 0.005              | 2.142  | -2.227 | -0.085              |
| 0.007              | 2.681  | -2.967 | -0.286              |
| 0.009              | 3.170  | -3.648 | -0.478              |
| 0.011              | 3.624  | -4.268 | -0.644              |
| 0.013              | 4.051  | -4.850 | -0.799              |
| 0.015              | 4.457  | -4.478 | -0.021              |
| 0.017              | 4.845  | -2.615 | 2.229               |
| 0.019              | 5.218  | 1.033  | 6.251               |
TABLE V: Internal energy (K) of spin polarized liquid $^3$He versus total number density at $\xi = 1/3$ computed with both microscopic calculation and using parabolic approximation.

| Density ($A^{-3}$) | Microscopic Calculation | Parabolic Approximation |
|--------------------|-------------------------|-------------------------|
| 0.003              | 0.096                   | 0.127                   |
| 0.005              | -0.268                  | -0.212                  |
| 0.007              | -0.688                  | -0.611                  |
| 0.009              | -1.135                  | -1.100                  |
| 0.011              | -1.532                  | -1.477                  |
| 0.013              | -1.444                  | -1.420                  |
| 0.015              | -0.523                  | -0.517                  |
| 0.017              | 1.685                   | 1.695                   |
| 0.019              | 5.667                   | 5.697                   |

TABLE VI: As Table V but for spin polarized liquid $^3$He at $\xi = 2/3$.

| Density ($A^{-3}$) | Microscopic Calculation | Parabolic Approximation |
|--------------------|-------------------------|-------------------------|
| 0.003              | 0.069                   | 0.124                   |
| 0.005              | -0.279                  | -0.164                  |
| 0.007              | -0.652                  | -0.488                  |
| 0.009              | -1.018                  | -0.867                  |
| 0.011              | -1.382                  | -1.164                  |
| 0.013              | -1.283                  | -1.186                  |
| 0.015              | -0.349                  | -0.331                  |
| 0.017              | 1.874                   | 1.895                   |
| 0.019              | 5.868                   | 5.891                   |
FIG. 1: Two-body correlation function of liquid $^3$He, $f(r)$, as a function of interatomic distance ($r$) at different values of spin asymmetry parameter $\xi = 0.0, 1/3, 2/3$ and 1.0 for $\rho = 0.01 \text{ A}^{-3}$. 
FIG. 2: Internal energy of liquid $^3\text{He}$ versus total number density at $\xi = 0.0$ (full curve), $1/3$ (dashed curve), $2/3$ (dotted curve) and $1.0$ (heavy dotted curve).
FIG. 3: Comparison of our results for the unpolarized (UnPol) and fully polarized (Pol) cases with the results of GFMC for different choices of the wave function. J refers to Jastrow, and J+T refers to Jastrow plus three-body wave functions \[12\].
FIG. 4: Comparison of our results for the unpolarized (UnPol) and fully polarized (Pol) cases with the results of FHNC [10]. J refers to Jastrow wave function.
FIG. 5: Comparison of our results for the unpolarized (UnPol) and fully polarized (Pol) cases with the results of FHNC [10]. J+T refers to Jastrow plus three-body wave function.
FIG. 6: Comparison of our results for the unpolarized (UnPol) and fully polarized (Pol) cases with the results of FHNC [10]. J+T+B refers to Jastrow plus three-body plus backflow wave function.