IJST (2015) 39A2: 199-204
Iranian Journal of Science & Technology

http://ijsts.shirazu.ac.ir

Ground state properties of liquid ^3He in the presence of magnetic field

G. H. Bordbar*, M. T. Mohammadi Sabet and M. Dehghani

Department of Physics, Shiraz University, Shiraz 71454, Iran
E-mail: ghbordbar@shirazu.ac.ir

Abstract

The ground state properties of liquid ^3He in the presence of magnetic field have been investigated. In our calculations, we have employed a variational many-body formalism using the Lennard-Jones and Aziz inter-atomic potentials. For this system, we have also computed the magnetization in magnetic fields up to 200 T. Our results show no ferromagnetic phase transition induced by the magnetic field. Here, a comparison has also been made between the results of the Lennard-Jones and Aziz potentials.

Keywords: Liquid ^3He; ground state properties; magnetic field; spin polarization

1. Introduction

Spin polarized liquid ^3He has been investigated by various authors in recent years (Castaing & Noziêres, 1979; Lhuillier & Laloe, 1982). In order to reach highly polarized liquid ^3He, the rapid melting and optical techniques have been proposed by Castaing and Noziêres (Castaing & Noziêres, 1979) and Lhuilier (Lhuillier & Laloe, 1982), respectively. Later, some theoretical approaches have been suggested to describe the polarized liquid ^3He microscopically (Gatica & Herna´ndez, 1998; Zong et al., 2003; Manouasakis et al., 1983; Glyde & Hernadi, 1984; Goudfrin et al., 2009; Wysokinski, et al., 2012; Wysokinski et al., 2014; Mishra, 1996). Also, phenomenological description based on Landau Fermi liquids theory has been used for spin polarized liquid ^3He (Sanchez-Castro et al., 1989; Bedell & Sanchez-Castro, 1986; Bedell, 1985). A new "metamagnetic" behavior of liquid ^3He has also been predicted (Sanchez-Castro et al., 1989). Study of magnetization of liquid ^3He predicts "nearly ferromagnetic" (Béal, 1983) and "nearly localized" (Vollhardt, 1984) models for spin polarized ^3He. The recent experimental data based on dynamical methods (Bravin et al., 1994; Bravin et al., 1992; Bravin et al., 1997; Buu et al., 2006) excluded these behaviors. These experiments show a downward curvature for magnetization curve of liquid ^3He up to $200\ T$.

Recently, we calculated the thermodynamic properties of spin polarized liquid ^3He using a many-body variational technique based on the cluster expansion of energy functional (Bordbar & Karimi, 2009; Bordbar, Karimi, & Mohsenipour, 2011; Bordbar & Karimi, 2011; Bordbar & Hoseini, 2012;). This method has led to good results for the bulk properties of liquid ^3He. Also, application of this method for the two dimensional liquid ^3He shows interesting results (Bordbar, Fatemi, & Mohammadi Sabet, 2013).

In the present study, we intend to investigate the ground state properties of liquid ^3He in the presence of magnetic field at zero temperature using the mentioned many-body variational method. In our calculations, we consider the Lennard-Jones (de Boer & Michels, 1939) and Aziz potentials (Aziz & et al., 1987) as the interaction between ^3He atoms.

2. Method

We consider a system of liquid ^3He with N interacting particles. In the presence of magnetic field, $N^{(+)}$ particles will be in spin-up state and $N^{(-)}$ particles will be in spin-down state. The polarization parameter of the system is defined as $\xi = \frac{N^{(+)}-N^{(-)}}{N}$, where $\xi = 1$ for the fully polarized case and $\xi = 0$ for unpolarized case. As mentioned in the previous section, we intend to calculate the properties of spin-polarized liquid ^3He in the presence of magnetic field using the variational method based on the cluster expansion of the

*Corresponding author
Received: 30 May 2014 / Accepted: 8 October 2014

energy. In this method, the trial wave function of N interacting particles is as follows,

$$\Psi(1,\dots,\mathrm{N}) = \mathrm{F}(1\dots\mathrm{N})\phi(1,\dots,\mathrm{N})$$

where $\phi(1,\dots,N)$ is the wave function of N non-interacting particles and $F(1,\dots,N)$ is a symmetric correlation function involving the whole effects of interaction between particles. In order to investigate the ground state properties of the system, we should calculate the total energy expectation value, $\langle H\rangle = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$. In the cluster expansion method, we consider the energy of the system up to the two-body cluster energy. Therefore, in the presence of magnetic field, the energy of liquid ^3He can be obtained from the following expression:

$$E = E_1 + E_2 + E_M \quad (1)$$

where E_1 and E_2 are the one-body and two-body energies, respectively, and E_M is the contribution of magnetic field in the total energy. We discuss the calculation of these contributions of the energy in the following subsections, separately.

2.1. One-body energy

The one-body energy per particle is given by

$$E_1 = E_1^{(+)} + E_2^{(-)} = \frac{3}{10}\left(\frac{\hbar^2}{2m}\right)(3\pi^2)^{2/3}\left[(1+\xi)^{5/3} + (1-\xi)^{5/3}\right]\rho^{2/3}, \quad (2)$$

where ρ is the total number density

$$\rho = \frac{N}{\Omega} = \rho^{(+)} + \rho^{(-)}. \quad (3)$$

2.2. Two-body energy

For the two-body energy per particle, we have,

$$E_2 = \frac{1}{2}\sum_{ij}\langle ij|W(12)|ij\rangle_a = \frac{1}{2}\sum_{ij}\langle ij|W(12)|ij-ji\rangle ,$$

where

$$\mathrm{W}(12) = -\frac{\hbar^2}{2\mathrm{m}}\left[\mathrm{F}(12),[\nabla_{12}^2,\mathrm{F}(12)]\right] + \mathrm{F}^{\dagger}(12)\mathrm{V}(12)\mathrm{F}(12) \quad (4)$$

is known as the effective potential. In the above equation, F(12) is the two-body correlation operator which in the Jastraw approximation (Bordbar & Karimi, 2009; Bordbar & Hoseini, 2012; Bordbar, Fatemi, & Mohammadi Sabet, 2013; Bordbar, Karimi, & Mohsenipour , 2011), it has the following form:

$$\mathrm{F}(12) = \mathrm{f}(\mathrm{r}_{12}) = \mathrm{f}(\mathrm{r}).$$

Using the Jastrow correlation function, we get the following relation for the effective potential:

$$W(12) = W(r) = \frac{\hbar^2}{m}(\nabla f(r))^2 + (f(r))^2 V(r) \quad (5)$$

In this relation $r = |\vec{r}_1 - \vec{r}_2|$, and $V(r)$ and $f(r)$ are the two-body potential and correlation function, respectively. In our calculations, we use the Lennard-Jones and Aziz potentials. Lennard-Jones potential is (de Boer & Michels, 1939)

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

where

$$\varepsilon = 10.22\,K, \quad \sigma = 2.556\ \text{Å}$$

The Aziz potential is as follows (Aziz & et al., 1987):

$$V(r) = \varepsilon\left\{Ae^{-\alpha r/r_m} - \left[C_6\left(\frac{r_m}{r}\right)^6 + C_8\left(\frac{r_m}{r}\right)^8 + C_{10}\left(\frac{r_m}{r}\right)^{10}\right]F(r)\right\}, \quad (7)$$

where

$$F(r) = \begin{cases} e^{-(\frac{D\,r_m}{r}-1)^2}, & \frac{r_m}{r} \le D \\ 1, & \frac{r_m}{r} > D \end{cases} \quad (8)$$

and

$\varepsilon = 10.8\,K$,
$A = 0.5448504\times10^6$,
$\alpha = 13.353384, r_m = 2.9673$ Å,
$C_6 = 1.37732412$,
$C_8 = 0.4253785$,
$C_{10} = 0.178100,\ D = 1.241314$.

After some algebra, we obtain the following relation for the two-body energy per particle,

$$E_2 = 2\pi\rho\int\left\{1 - \frac{1}{4}\left[(1+\xi)^2 l^2\left(k_F^{(+)}r\right) + (1-\xi)^2 l^2\left(k_F^{(-)}r\right)\right]\right\}W(r)r^2dr , \quad (9)$$

where

$$l\left(x^{(i)}\right) = \frac{3}{(x^{(i)})^3}\left[\sin\left(x^{(i)}\right) - x^{(i)}\cos\left(x^{(i)}\right)\right], \quad (10)$$

is called statistical correlation function, and

$$k_F^{(+)} = [6\pi^2\rho^{(+)}]^{1/3}, \quad k_F^{(-)} = [6\pi^2\rho^{(-)}]^{1/3}, \quad (11)$$

are the Fermi momentum of spin-up and spin-down states, respectively. $L^2(r)$ is defined as follows:

$$L^2(r) = 1 - \frac{1}{4}\left[(1+\xi)^2 l^2\left(k_F^{(+)}r\right) + (1-\xi)^2 l^2\left(k_F^{(-)}r\right)\right]. \quad (12)$$

By minimizing the two-body energy (Eq. (8)) with respect to the variation in two-body correlation function subject to the normalization constraint,

$$\frac{1}{N}\sum_{ij}\langle ij|h^2(12)-f^2(12)|ij\rangle_a = 1\,, \qquad (13)$$

where $h(12)=h(r)=\frac{1}{L(r)}$ is called Pauli function, we obtain the following Euler-Lagrange differential equation,

$$f''(r)L(r)+2f'(r)L'(r)-\frac{m}{\hbar^2}(V(r)-2\lambda)f(r)L(r)=0\,. \qquad (14)$$

The two-body correlation function $f(r)$ is obtained by numerically integrating this equation. Using this two-body correlation function, the two-body energy E_2 can be calculated.

2.3. Magnetic energy

The contribution of magnetic energy, E_M, is as follows:

$$E_M = -\sum_{i=1}^{N}\vec{\mu}_i.\vec{B}\ , \qquad (15)$$

where $\mu=-1.074490695\times10^{-26}\,JT^{-1}$ is the magnetic dipole moment of the ^3He atoms. We consider the external magnetic field, $\vec{B}$, along $\vec{B}$ axis ($\vec{B}=B\hat{z}$). Therefore, we have

$$E_M = -\sum_{i=1}^{N}\vec{\mu}_i.\ \vec{B}=-\mu\left[N^{(+)}-N^{(-)}\right]B\ . \qquad (16)$$

Finally, the magnetic energy per particle is given by

$$\frac{E_M}{N}=-\mu\left[\frac{N^{(+)}-N^{(-)}}{N}\right]B=-\mu\xi B \qquad (17)$$

3. Results and Discussion

In Fig. 1, the energy per particle (Eq. (1)) of polarized liquid ^3He has been shown versus spin polarization parameter for different values of magnetic field at densities 0.005 and 0.015Å^{-3} for the Lennard-Jones and Aziz potentials. We have found that for the Lennard-Jones potential, at magnetic fields less than $100\,T$, the energies calculated are nearly identical. This means that in the case of Lennard-Jones potential, in this range, the magnetic field has no substantial effects on the energy of system. However, we see that in the case of Aziz potential, the influence of magnetic field on the energy for the values less than $100\,T$ is considerable. A Comparison between the energy curves in Fig. 1 shows that by applying the magnetic field, for both employed interatomic potentials, the minimum value of energy (the ground state energy) appears in negative polarizations ($-1<\xi<0$). From Fig. 1, we see that by increasing the magnetic field, for each density, the ground state energy decreases. This means that the increasing magnetic field leads to a more stable state for the system.

We have compared the energy per particle of liquid ^3He calculated by both Lennard-Jones and Aziz potentials for two different densities at magnetic field $B=100\,T$ in Fig. 2. It is clear that for the Lennard-Jones potential, the energy per particle at different densities and magnetic fields is lower than that for the Aziz potential. In fact, the system is more stable for the case of Lennard-Jones potential.

In Fig. 3, the spin polarization parameter corresponding to the ground state of the system has been plotted versus density for different values of magnetic field. As it is observed for each value of magnetic field, the magnitude of spin polarization parameter decreases by increasing density, except around the density range in which the energy versus density has a minimum point (Bordbar & Karimi, 2011; Bordbar & Karimi, 2009). We see that for the Lennard-Jones (Aziz) potential at density $\rho=0.013\text{Å}^{-3}$ ($\rho=0.013\,\text{Å}^{-3}$), the spin polarization parameter reaches a minimum, especially for high magnetic fields. This figure also shows that at each density, the spin polarization parameter increases by increasing the magnetic field.

The magnetization of the system can be obtained using the following relation:

$$M=-\left(\frac{\partial E}{\partial B}\right)_{\rho}\,. \qquad (18)$$

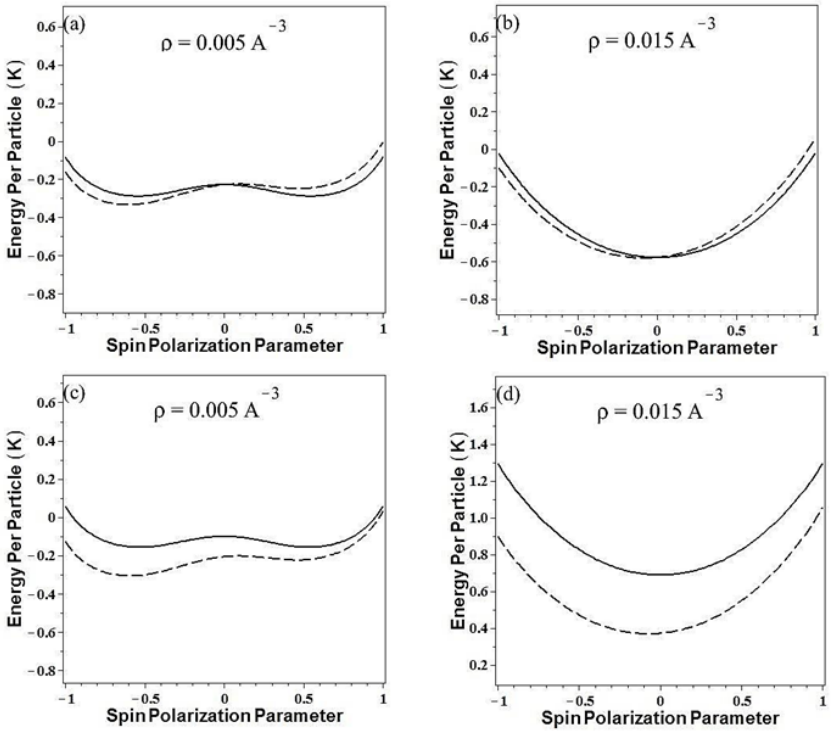

Fig. 1. The energy per particle versus the spin polarization parameter (ξ) for the magnetic fields B=0 (full curve) and 100 (dashed curve) with the Lennard-Jones (a,b) and Aziz (c,d) potentials at ρ=*0.005* and 0.015 A^{-3}

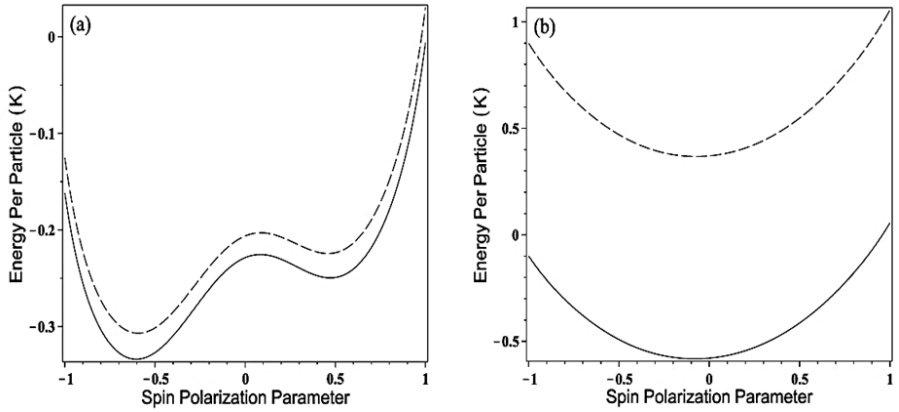

Fig. 2. The energy per particle versus the spin polarization parameter (ξ) with the Lennard-Jones (full curve) and Aziz (dashed curve) potentials at ρ=*0.005* (a) and 0.015 A^{-3} (b)

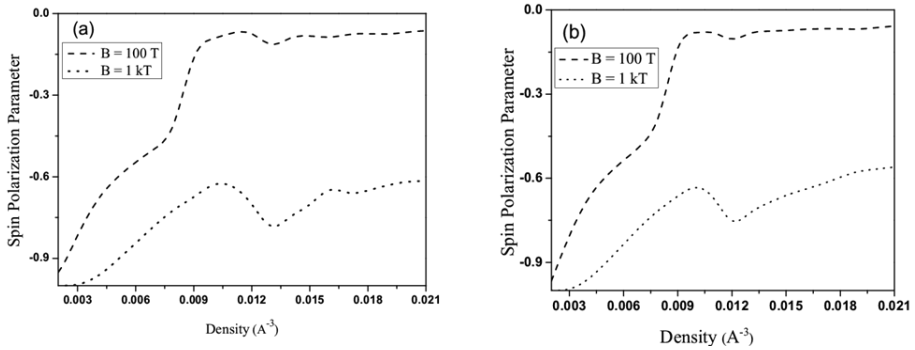

Fig. 3. The spin polarization parameter corresponding to the equilibrium state of system as a function of density at different values of magnetic field (*B*) with the Lennard-Jones (a) and Aziz (b) potentials

We have calculated the magnetization of spin polarized liquid ^3He for the magnetic fields up to $200\,T$. Our results for the magnetization $(\frac{M}{N|\mu|})$ versus magnetic field have been plotted in Fig. 4. We see from this figure, as it is expected (Gatica & Herna´ndez, 1998; Buu et al., 2006), at low magnetic fields, the magnetization versus magnetic field is linear. Figure 4 shows that at high magnetic fields, the magnetization has a downward curvature, and therefore it has a monotonic increasing slope which excludes a metamagnetic instability. Our results are overally in a good agreement with those of others (Buu et al., 2006; Bravin et al., 1992; Bravin et al., 1994; Bravin et al., 1997; Buu & et al., 2006). In the panel (c) of Fig. 4, we have shown the experimental results (Gatica & Herna´ndez, 1998). As we see from this Fig., the general behavior of our magnetization curve versus magnetic field is similar to that of experiment. However, the magnitude of the magnetization extracted by experimental data is greater than our result. The main reason for this difference is that the experimental data has been obtained at constant pressure whereas we have done our calculation at constant density. Of course, our results can be improved if we consider the effects of three-body cluster energy and the spin-spin correlation in our calculations (Bordbar & Mohammadi Sabet, 2015).

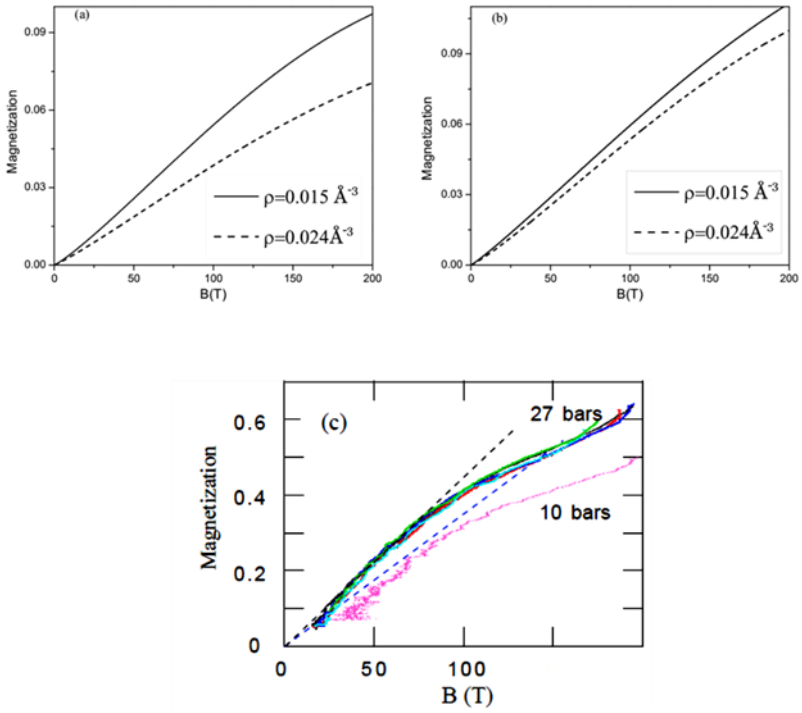

Fig 4. The magnetization ($\frac{M}{N\,|\,\mu|}$) as a function of magnetic field at different densities (ρ) with the Aziz (a) and Lennard-Jones (b) potentials. The experimental results (c) have also been given for comparison (Gatica & Herna´ndez, 1998)

4. Summary and Conclusions

In this article, we have studied the magnetization of spin polarized liquid ^3He in the presence of magnetic field at zero temperature using variational method. It was found that for the Lennard-Jones potential, the magnetic fields less than $100\,T$ have no considerable effects on the energy of the system, while this effect for the case of Aziz potential is substantial. Also, it was shown that in the presence of magnetic field, the spin polarization symmetry is broken, and the minimum of energy occurs at $-1 < \xi < 0$. It is seen that the effect of magnetic field on the polarization of liquid ^3He at low polarizations is more noticeable. We have shown that the magnetization of liquid ^3He, in general, has a downward curvature. Therefore, the magnetization increases monotonically with increasing the magnetic field. This shows no ferromagnetic phase transition in the liquid ^3He. There is an overal agreement between our results and the experimental data and the density functional results (Buu & et al., 2006; Bravin & et

al., 1992; Bravin & et al., 1994; Bravin & et al., 1997; Buu & et al., 2006).

Acknowledgments

We wish to thank Shiraz University research council.

References

Aziz, R., & et al. (1987). A new determination of the ground state interatomic potential for ^3He. *Mol. Phys.*, 61, 1487–1511.

Béal, M. (1983). Field dependences of magnetization and specific-heat coefficient in a nearly magnetic system: Liquid ^3He and strong Pauli Paramag. *Phys. Rev. B*, 27, 4467–4470.

Bedell, K., & Sanchez-Castro, C. (1986). Near-metamagnetism of liquid ^3He at high pressure. *Phys. Rev. B*, 57, 854–857.

Bedell, K. (1985). Pressure changes and magnetostriction in finite magnetic fields in ^3He and other normal Fermi liquids. *Phys. Rev. Lett.*, *54*, 1400–1403.

Bordbar, G., & Hoseini, S. (2012). Isentropic calculations for normal liquid ^3He using the lowest order constrained variational method. *IJST, Trans. A, 36*, 225–230.

Bordbar, G., & Karimi, M. (2009). LOCV calculations for polarized liquid ^3He with the spin-dependent correlations. *Int. J. Mod. Phys. B, 23*, 2373–2382.

Bordbar, G., & Karimi, M. J. (2011). Variational Calculations for normal liquid ^3He at finite temperature using the spin-dependent correlation function. *Int. J. Mod. Phys. B, 25*, 4359–4368.

Bordbar, G., & Mohammadi Sabet, M. (2015). A Variational calculation of magnetized correlated fermion system using a spin-dependent correlation: application to liquid ^3He. *Int. J. Mod. Phys. B, 29*, 1550046–1550059.

Bordbar, G., Fatemi, F., & Mohammadi Sabet, M. T. (2013). Lowest order constrained variational calculation for two-dimensional liquid ^3He. *J. Theor. Comput. Chem., 12*, 1350061–1350071.

Bordbar, G., Karimi, M., & Mohsenipour, S. (2011). LOCV calculations for polarized liquid ^3He: The effect of three-body cluster energy. *Int. J. Mod. Phys. B, 25*, 2355–2363.

Bravin, M., et al. (1992). A high field squid magnetometer for studying spin-polarized liquid ^3He. *J. Low Temp. Phys., 98*, 723–726.

Bravin, M., et al. (1994). Measurements of the nuclear magnetism of liquid ^3He up to 25 Tesla using a torque magnetometer. *Physica B, 194–196*, 745–746.

Bravin, M., et al. (1997). Thermodynamic measurement of the magnetization curve of liquid ^3He up to 200 Tesla. *Physica B, 197*, 410–416.

Buu, O., et al. (2006). *Progress in Low Temperature Physics.* (W. Halperin, Ed.) New York: Science direct.

Castaing, B., & Noziêres, P. (1979). Phase transitions of spin polarized ^3He: a thermodynamical nuclear orientation technique ? *J. Phys. (Paris), 40*, 257–268.

de Boer, J., & Michels, A. (1939). Quantum-mechanical calculation of the second virial-coeficient of helium at low temperatures. *Physica, 6*, 409–420.

Gatica, S., & Herna´ndez, E. (1998). Spin-polarized ^3He in a density-functional frame. *Phys. Rev. B, 58*, 12300–12306.

Glyde, H., & Hernadi, S. (1984). Fully-spin-polarized ^3He. *Phy. Rev. B, 29*, 3873–3880.

Goudfrin, V., & et al. (2009). Magnetic susceptibility of liquid ^3He. *J. Phys. Conference Series, 150*, 032024–032028.

Lhuillier, C., & Laloe, F. (1982). Transport properties in a spin-polarized gas. *J. Phys. (Paris), 43*, 192–225.

Manouasakis, E., et al. (1983). Microscopic calculations for normal and polarized liquid ^3He. *Phy. Rev. B, 28*, 3770–3781.

Mishra, S. (1996). Field dependence of magnetization in liquid ^3He. *Physica B, 223-224*, 637–639.

Sanchez-Castro, C., & et al. (1989). Spin-polarized Fermi liquids: Applications to liquid ^3He. *Phys. Rev. B, 40*, 437–453.

Vollhardt, D. (1984). Normal ^3He: an almost localized Fermi liquid. *Rev. Mod. Phys., 56*, 99-120.

Wysokinski, M., & et al. (2012). Magnetic and thermodynamic properties of correlated fermions - application to liquid ^3He. *AIP Conf. Proc., 1485*, 319–323.

Wysokinski, M., et al. (2014). Properties of an almost localized Fermi liquid in an applied magnetic field revisited: a statistically consistent Gutzwiller approach. *J. Phys: Cond. Matt., 26*, 055601.

Zong, F. H. et al. (2003). The polarization energy of normal liquid ^3He. *Mol. Phys., 101*, 1705–1711.