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EFFECT OF THREE-BODY CLUSTERS IN THE GROUND-STATE PROPERTIES OF SPIN-POLARIZED LIQUID ^{3}He

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The ground-state energy of polarized and unpolarized liquid ^{3}He is calculated using the variational theory. A variational wave function is constrained to be normalized appropriately by including the three-body terms in the cluster expansion of the two-body radial distribution function. The higher-order terms have been found to be important to obtain an equation of state which is in agreement with experimental data. The saturation density of unpolarized liquid ^{3}He was found to be $0.267\sigma^{-3}$, which decreases by enhancing the polarization. For all relevant densities, the ground-state energy of the spin-polarized system is higher than that in the unpolarized case.

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1. INTRODUCTION

Liquid ^{3}He is an interesting system in which many-body correlations play an important role in determining its properties [1]. This system obeys Fermi–Dirac statistics the same as neutron stars, whereas describing ^{3}He is easer than neutron stars because of the simplicity of inter-particle interaction. Moreover, we have accumulated a huge amount of experimental information about ^{3}He. Hence, for theoreticians, liquid ^{3}He can be considered an excellent laboratory to test many-body theories applied to neutron stars.

Experimentally, the zero-temperature equation of state of liquid ^{3}He is known and the density of equilibrium is $\rho_0 = 0.277\sigma^{-3}$ with $\sigma = 2.556$ Å [2]. Theoretically, most of the available many-body methods have been applied for investigating the properties of liquid ^{3}He, two successful approaches are Fermi hypernetted-chain (FHNC) and quantum Monte Carlo (QMC) methods. Viviani et al. used a variational wave function which includes pair, triplet, backflow, and spin dependent correlations in the FHNC method to obtain an equation of state which is in very close agreement with the experimental data [3]. Casulleras and Boronat in 2000, using optimized backflow correlations, applied the diffusion Monte Carlo (DMC) method and generated an equation of state of liquid ^{3}He which is in excellent agreement with experimental data from equilibrium up to freezing [4]. In 2003, this computation was revisited by using exactly the same potential, wave function, and number of particles as used by Casulleras and Boronat, but their results were not confirmed [5].

In addition, in 1979 liquid ^{3}He was polarized by a rapid melting of a highly polarized solid ^{3}He [6]. In this state, nuclear spins of ^{3}He aligned and because of nuclear magnetic interaction, the intrinsic relaxation time of partially polarized ^{3}He is long, which allows using it for magnetic resonance imaging [7]. Most of the theoretical investigations based on QMC predict the fully polarized state with a lower energy than for the unpolarized state [8, 9]. By considering backflow and three-body wave functions and twist-averaged boundary conditions in the QMC approach, it was found that the energy of the polarized state was higher than the unpolarized one, but the obtained susceptibility had discrepancy with extrapolated experimental data [5, 10]. Manosuki et al., by using the FHNC technique, found that the energy of spin-polarized phase was above that of the normal phase [11]. They conclude that the three-body and backflow correlations are very important for their variational wave function. They predicted that this system could exhibit new phase transitions to ferromagnetism, while no such new phase has been discovered so far.

The lowest-order constrained variational (LOCV) method is a many-body approach which has been developed to study the bulk properties of the quantum

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fluids [12–14]. In recent years, this method has been applied to study homogeneous normal liquid ^{3}He [15–18]. In this variational approach, as we see in the next section, we use a cluster expansion to calculate the energy and other properties of system. Convergence of the expansion and the effect of higher-order cluster terms in the energy of unpolarized liquid ^{3}He was studied and it has been shown that higher-order cluster terms in the normalization constraint improve the equation of state [14]. The LOCV method has several advantages with respect to the other many body methods which go beyond the lowest order [14]. Two of them are: (i) the LOCV method is fully self-consistent, i. e., there are no free parameters in this variational approach. (ii) It considers a particular form for the long-range part of the correlation function in order to perform an exact functional minimization of the energy. It is shown that correlation functions obtained from the extended LOCV (ELOCV) lead to more accurate results for the momentum distribution [19, 20], ^{3}He droplets [21], and ^{3}He atoms in nanotube [22]. In a series of papers, Bordbar et al. applied the LOCV method to the polarized case and calculated some properties of this system [18, 23–25]. In their recent work, they considered the ground-state properties with the three-body cluster contributions [26]. But they did not consider the effect of three-body cluster expansion of the two-body radial distribution function (ELOCV). We expect that the same as in QMC and FHNC methods, three-body correlations are very important in spin-polarized systems. Hence, in this paper, we intend to consider the effect of higher-order terms in the cluster expansion of the radial distribution function and calculate the energy by the extended LOCV approach with the three-body cluster contributions.

2. SCHEME OF CALCULATIONS

2.1. Cluster expansion of energy

The Hamiltonian of the normal liquid ^{3}He consists of N atoms interacting with each other and is usually written as

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2}\sum_{i\neq j} V(ij), \qquad (2.1)$$

where $V(ij)$ is the two-body inter-atomic potential. In this work, we use the Lennard–Jones potential. In the LOCV method, we use an ideal Fermi gas type wave function (ϕ) for single-particle states to find the variational wave function of the interacting system:

$$\psi_v = F\phi, \qquad (2.2)$$

where F is a correlation function which incorporates the correlations induced by interactions. To calculate the energy expectation value, we use the variational principle and a cluster expansion developed in Ref. [27],

$$E([f]) = \frac{1}{N}\frac{\langle\psi_v|H|\psi_v\rangle}{\langle\psi_v|\psi_v\rangle} = E_1 + E_2 + E_3 + \ldots \qquad (2.3)$$

The one-body term E_1 is just the familiar Fermi-gas kinetic energy, i. e.,

$$E_1 = \frac{1}{N}\sum_{i=1}^{N} \left\langle i \left| \frac{\hbar^2 k_i^2}{2m} \right| i \right\rangle . \qquad (2.4)$$

The two-body energy E_2 is

$$E_2 = \frac{1}{2N}\sum_{ij} \langle ij|W(12)|ij\rangle_a \qquad (2.5)$$

and the "effective interaction operator" $W(12)$ is given by

$$W(12) = \frac{\hbar^2}{m}(\nabla f(12))^2 + f^2(12)V(12), \qquad (2.6)$$

where $f(12)$ and $V(12)$ are the two-body correlation and inter-atomic potential.

Higher-order correlations are considered in terms of statistically irreducible two-body correlations. So, the three-body energy is written as

$$E_3 = E_{3h} + E_{3hh} + E_{3t}, \qquad (2.7)$$

where

$$E_{3h} = \frac{1}{N}\sum_{ijk} [\langle ijk|h(13)W(12)|ijk\rangle_a - \\ - \langle ik|h(13)|ik\rangle_a \langle ij|W(12)|ij\rangle_a], \qquad (2.8)$$

$$E_{3hh} = \frac{1}{2N}\sum_{ijk} \langle ijk|h(13)h(23)W(12)|ijk\rangle_a, \qquad (2.9)$$

$$E_{3t} = \frac{1}{2N} \times \\ \times \sum_{ijk} \left\langle ijk \left| \frac{\hbar^2}{4m} f^2(31)\nabla_2 h(12)\nabla_2 h(23) \right| ijk \right\rangle_a , \qquad (2.10)$$

and

$$h(ij) = f^2(ij) - 1. \qquad (2.11)$$

We note that in Eq. (2.3), to collect all contributions which are conventionally assigned to the first order in the smallness parameter, we have to compute a special portion of the four-body terms, like the three-body cluster terms [27]:

$$E_{4h} = \frac{1}{4N}\sum_{ijkl}\langle ij|h(34)|kl\rangle_a \langle kl|W(12)|ij\rangle_a. \qquad (2.12)$$

In the LOCV formalism we constrain the two-body correlation function to normalize the wave function of the system. We hope this constraint makes the cluster expansion converge very rapidly.

2.2. Spin polarized calculations

We now specialize the above cluster expansion to the spin-polarized system including N atoms with $N^{(+)}$ spins up and $N^{(-)}$ spins down, with

$$\rho = \frac{N}{\Omega} = \rho^{(+)} + \rho^{(-)} \qquad (2.13)$$

being the total number density and the spin asymmetry parameter ζ defined as

$$\zeta = \frac{N^{(+)} - N^{(-)}}{N}. \qquad (2.14)$$

By considering the single-particle states $|i\rangle$ as plane waves, we can calculate the energy terms introduced in the last section. The one-body energy term E_1 is

$$E_1 = \frac{3}{10}\frac{\hbar^2}{2m}(3\pi^2\rho)^{2/3}[(1+\zeta)^{5/3}+(1-\zeta)^{5/3}]. \qquad (2.15)$$

The two-body energy E_2 introduced in Eq. (5) is

$$E_2 = 2\pi\rho\int r_{12}^2 dr_{12}\left[1 - \frac{1}{4}(1+\zeta)^2\ell^2(k_F^{(+)}r_{12}) - \right.$$
$$\left. - \frac{1}{4}(1-\zeta)^2\ell^2(k_F^{(-)}r_{12})\right] W(r_{12}), \qquad (2.16)$$

where

$$\ell(x) = 3\frac{j_1(x)}{x} = \frac{3}{x^3}(\sin(x) - x\cos(x)) \qquad (2.17)$$

is called the statistical correlation function or the Slater factor [28]; $k_F^{(+)} = (6\pi^2\rho^{(+)})^{1/3}$ and $k_F^{(-)} = (6\pi^2\rho^{(-)})^{1/3}$ are the Fermi momenta of spin up and spin down states, respectively.

The three-body cluster energies in Eqs. (8), (9), and (10) are

$$E_{3h} = \frac{\rho^3}{8N}\times$$
$$\times\int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 h(r_{13})W(r_{12})\Gamma_1(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3), \qquad (2.18)$$

$$E_{3hh} = \frac{\rho^3}{2N}\int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 h(r_{13})\times$$
$$\times W(r_{12})h(r_{23})\Gamma_2(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3), \qquad (2.19)$$

$$E_{3t} = \frac{\rho^3}{2N}\int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 \frac{\hbar^2}{4m}\times$$
$$\times f^2(r_{31})\nabla_2 h(r_{12})\nabla_2 h(r_{23})\Gamma_2(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3). \qquad (2.20)$$

Here, the three-body energy terms $\Gamma_1(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$ and $\Gamma_2(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$ are defined as follows:

$$\Gamma_1(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) =$$
$$= (1+\zeta)^3\ell(k_F^{(+)}r_{12})\ell(k_F^{(+)}r_{23})\ell(k_F^{(+)}r_{31}) +$$
$$+ (1-\zeta)^3\ell(k_F^{(-)}r_{12})\ell(k_F^{(-)}r_{23})\ell(k_F^{(-)}r_{31}) -$$
$$- [(1+\zeta)^3 + (1+\zeta)^2(1-\zeta)]\ell^2(k_F^{(+)}r_{23}) -$$
$$- [(1-\zeta)^3 + (1-\zeta)^2(1+\zeta)]\ell^2(k_F^{(-)}r_{23}) \qquad (2.21)$$

and

$$\Gamma_2(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = 1 - \frac{1}{8}[(1+\zeta)^3 + (1+\zeta)^2(1-\zeta)]\times$$
$$\times [\ell^2(k_F^{(+)}r_{12}) + 2\ell^2(k_F^{(+)}r_{23})] -$$
$$-\frac{1}{8}[(1-\zeta)^3+(1-\zeta)^2(1+\zeta)][\ell^2(k_F^{(-)}r_{12})+2\ell^2(k_F^{(-)}r_{23})]+$$
$$+ \frac{1}{4}(1+\zeta)^3\ell(k_F^{(+)}r_{12})\ell(k_F^{(+)}r_{23})\ell(k_F^{(+)}r_{31}) +$$
$$+ \frac{1}{4}(1-\zeta)^3\ell(k_F^{(-)}r_{12})\ell(k_F^{(-)}r_{23})\ell(k_F^{(-)}r_{31}). \qquad (2.22)$$

And finally,

$$E_{4h} = \frac{1}{32N}\rho^4\int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 d\mathbf{r}_4 h(r_{34})W(r_{12})\times$$
$$\times \{(1+\zeta)^4[\ell^2(k_F^{(+)}r_{13})\ell^2(k_F^{(+)}r_{24}) - \ell(k_F^{(+)}r_{31})\times$$
$$\times \ell(k_F^{(+)}r_{23})\ell(k_F^{(+)}r_{14})\ell(k_F^{(+)}r_{24})] +$$
$$+ (1-\zeta)^4[\ell^2(k_F^{(-)}r_{13})\ell^2(k_F^{(-)}r_{24}) - (\ell(k_F^{(-)}r_{31})\times$$
$$\times \ell(k_F^{(-)}r_{23})\ell(k_F^{(-)}r_{14})\ell(k_F^{(-)}r_{24})]\}. \qquad (2.23)$$

The above terms can be simplified by putting particle 1 at the origin and replacing $\rho\int d\mathbf{r}_1 = N$.

2.3. Normalization constraint and the Euler–Lagrange equation

Now, we minimize the energy with respect to $f(r)$, whereas in LOCV formalism we are interested in obtaining a more physical correlation function that satisfies the normalization constraint $\langle\psi_v|\psi_v\rangle = 1$. In the lowest-order approximation, this constraint is given by [28]

$$\rho \int (g_2(r_{12}) - 1)\, d^3r_{12} = -1, \tag{2.24}$$

where $g_2(r_{12})$ is the two-body radial distribution function, which has the cluster expansion

$$g_2(r_{12}) = f^2(r_{12}) \sum_{n=2}^{N} [\Delta g(r_{12})]_n. \tag{2.25}$$

The first two terms of above expansion are

$$[\Delta g(r_{12})]_2 = g_F(r_{12}) \tag{2.26}$$

and

$$\begin{aligned} [\Delta g(r_{12})]_3 &= \frac{1}{4}\rho \int d^3r_3 h(r_{13}) \Gamma_1(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) + \\ &+ \rho \int d^3r_3 h(r_{13}) h(r_{23}) g_{3F}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3), \end{aligned} \tag{2.27}$$

where $g_F(r_{12})$ and $g_{3F}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)$ are the two- and three-body radial correlation functions of the noninteracting Fermi gas ground state,

$$\begin{aligned} g_F(r_{12}) = 1 &- \frac{1}{4}(1+\zeta)^2 \ell^2(k_F^+ r) - \\ &- \frac{1}{4}(1-\zeta)^2 \ell^2(k_F^- r), \end{aligned} \tag{2.28}$$

$$g_{3F}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \Gamma_2(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3).$$

In most of the previous calculations, based on the LOCV method, only the $n = 2$ term was included in the two-body distribution function, Eq. (2.25). But in the extended version of the lowest-order constrained variational formalism (ELOCV) applied in this work, we extend the above cluster expansion to the $n = 3$ term. In other words, the ELOCV formalism leads to a more accurate variational wave function, so that the normalization constraint is satisfied more properly. So, we expect our obtained wave function and the pair radial distribution function to be more physical.

The normalization constraint, Eq. (2.24), introduces another parameter into our formalism, i. e., the Lagrange multiplier λ. By using the Euler–Lagrange equation, we minimize the functional $L(r, f, f') = r^2\{E + \lambda\langle\psi_v|\psi_v\rangle\}$ with respect to $f(r)$ and we choose λ such that the above normalization constraint is satisfied, i. e.,

$$\frac{\partial L}{\partial r} - \frac{\partial}{\partial r}\frac{\partial L}{\partial f'(r)} = 0. \tag{2.29}$$

We solve this equation to find correlation functions and the ground-state energy of spin polarized liquid ^{3}He. Note that in LOCV formalism, in contrast to other variational approaches, we set the correlation function equal to the Pauli function instead of 1 [15].

3. RESULTS AND DISCUSSION

The obtained two-body correlation functions for fully polarized ($\zeta = 1$ situation) and unpolarized ($\zeta = 0$ situation) liquid ^{3}He are shown in Fig. 1. This figure shows that the correlation function for the fully polarized case, especially the correlation function of the ELOCV formalism, tends to the Pauli function more rapidly than unpolarized one. So, when atom spins are aligned with each other, they have a shorter correlation length than in a misaligned state. The calculated two-body radial distribution functions introduced in Eq. (2.25) are plotted in Fig. 2 for fully polarized and unpolarized liquid ^{3}He. It is clear that including the $n = 3$ term leads to better results.

We have plotted the equation of state results of LOCV and ELOCV calculations for unpolarized liq-

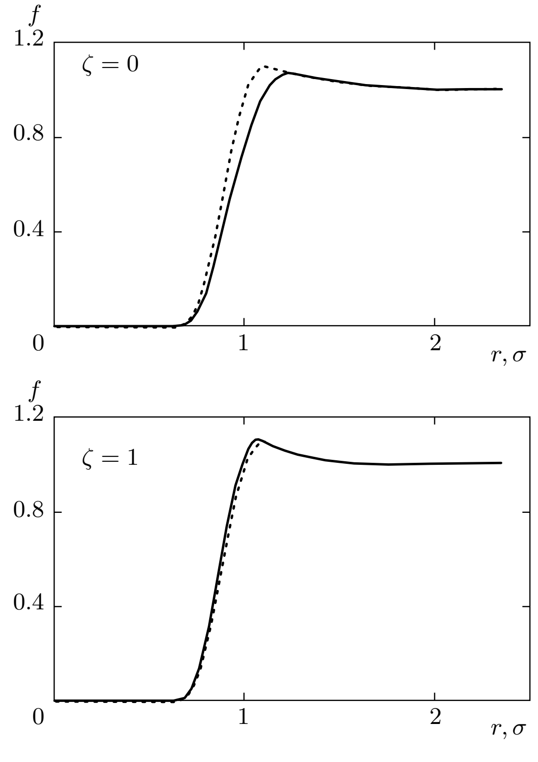

Fig. 1. ELOCV (solid lines) and LOCV (dashed lines) correlation functions of unpolarized ($\zeta = 0$) and fully polarized ($\zeta = 1$) liquid ^{3}He at $\rho = 0.277\sigma^{-3}$

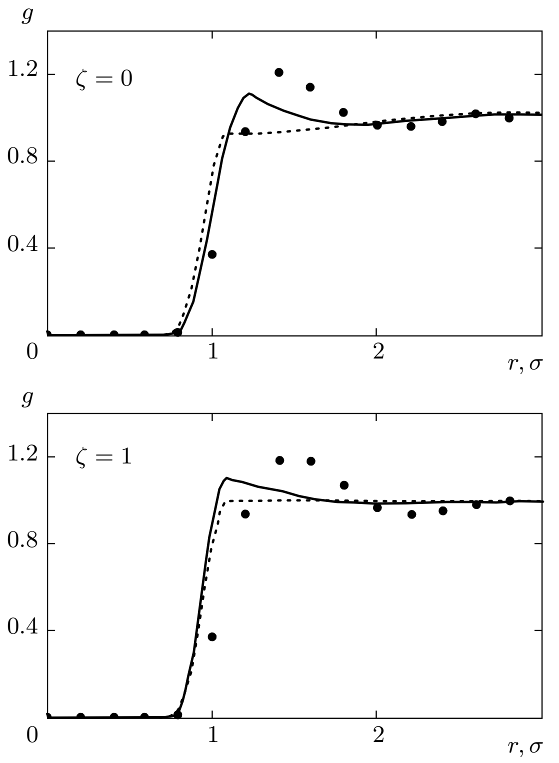

Fig. 2. Comparison of our ELOCV (solid lines) and LOCV (dashed lines) two-body radial distribution functions with the FHNC method (circles) [11] for unpolarized ($\zeta = 0$) and fully polarized ($\zeta = 1$) liquid ^{3}He at $\rho = 0.277\sigma^{-3}$

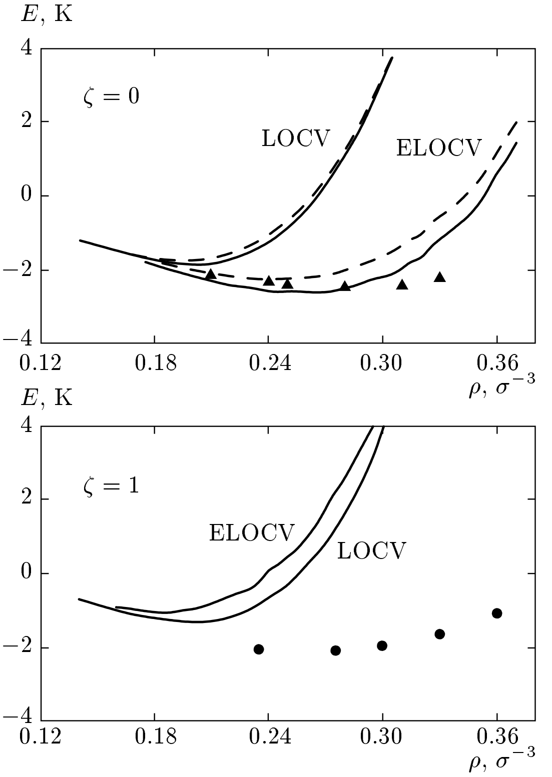

Fig. 3. Comparison of our calculated ground-state energy of unpolarized ($\zeta = 0$) and fully polarized ($\zeta = 1$) liquid ^{3}He with experiment [2] and FHNC results [11]. Solid lines and dashed lines represent energy with and without the contribution of the three-body cluster energy E_3, respectively

Table. Saturation density and equilibrium energy of unpolarized liquid ^{3}He

	LOCV	ELOCV	Experiment
ρ_0, σ^{-3}	0.205	0.267	0.277
E_0, K	−1.88	−2.61	−2.47

uid ^{3}He ($\zeta = 0$ situation) as a function of the density in Fig. 3. To see the effect of the three-body energy, Eq. (2.7), we present results with and without the three-body cluster energy. The experimental data [2] are also given for comparison. As we see, the ELOCV results are closer than the LOCV ones to the experimental data. In both cases, the three-body energy improves the results. As we explained in the preceding section, in the ELOCV calculation, we insert the radial distribution function, Eq. (2.25), in the normalization constraint, Eq. (2.24), up to the three-body cluster term.

Our binding energies E_0 at the equilibrium density ρ_0 obtained from the LOCV and ELOCV approaches with the three-body cluster energy are tabulated in the Table. In comparison with experimental values, there is good agreement between the ELOCV and experiment.

In Fig. 3, we also show the energy of fully polarized ($\zeta = 1$) liquid ^{3}He as a function of liquid densities for the LOCV and ELOCV approaches separately. This figure indicates that as polarization increases, the energy takes higher values and there is no crossing point between the energy curves of polarized and unpolarized cases. This behavior is in agreement with experiment. The equilibrium density and the polarization energy do not vary with density considerably, in the LOCV case. But in the ELOCV situation, the equilibrium density decreases and polarization energy increases with increasing spin polarization. Because of the Pauli exclusion principle, we expect that when fermions such as ^{3}He atoms are polarized, they exclude each other and so the density decreases with increasing the pola-

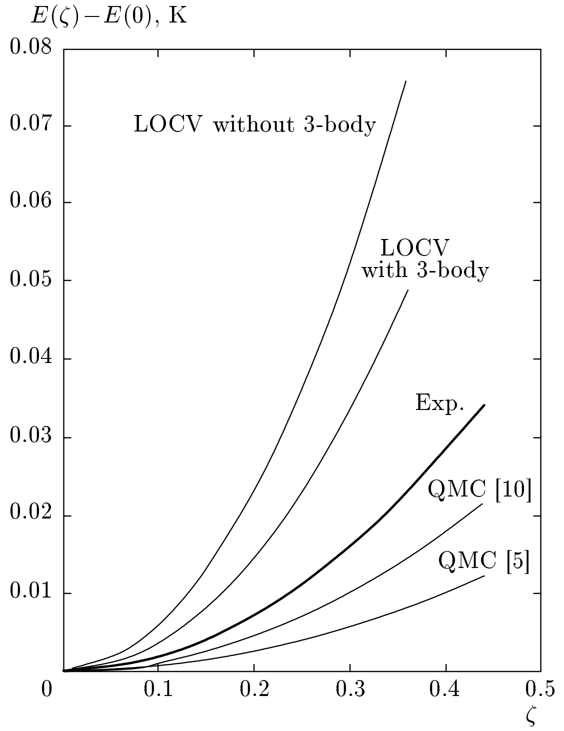

Fig. 4. Polarization energy versus spin polarization of liquid ^{3}He at the experimental equilibrium density. QMC [5, 10] and experimental [29] curves are a fit of data using a quadratic polynomial

rization parameter, the same as ELOCV results.

To investigate the effect of spin polarization on the polarization energy, in Fig. 4 we plot our computed energy at the experimental equilibrium density $\rho_0 = 0.277\sigma^{-3}$ versus polarization of ^{3}He. We have shown the extrapolations of experimental [29] and QMC [5, 10] method data obtained by assuming $E = E_0 + \zeta^2/(2\chi/C)$ for the relation between energy and the spin polarization parameter. This figure shows that the contribution of the three-body energy makes the curve of the LOCV formalism closer to the experimental curve.

In conclusion, in this paper, we have extended LOCV calculations to include the three-body contributions. We find that the three-body correlations improve the radial distribution function, the equation of state, and the polarization energy of liquid ^{3}He. It is found that as the polarization of liquid ^{3}He increases, the two-body correlation length becomes shorter. The obtained results show that the internal energy of liquid ^{3}He increases with increasing the spin asymmetry parameter with no crossing point between polarized and unpolarized energy curves. It is also seen that there is a bound state for polarized liquid ^{3}He. Our results indicate that in the framework of cluster expansion, the role of the normalization constraint is very important in many-body calculations, and higher-order normalization leads to more physical results. In the QMC [5, 10] and FHNC [11] methods, besides the three-body effect, the backflow effect is also included. In (E)LOCV, it is possible to consider this effect by choosing the momentum-dependent correlation function and obtain new equations for energy terms. We expect that the backflow effect has some effects in both polarized and unpolarized cases, but we leave it for future work.

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