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Lowest order constrained variational method applied to liquid ^{3}He

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Abstract. The energy of normal liquid ^{3}He is obtained using the lowest order constrained variational (LOCV) method. In order to test the convergence of the cluster expansion series, the three-body cluster energy is calculated, with the LOCV correlation functions, and by imposing the normalization constraint on the two-body distribution function which includes three-body cluster correlations (LOCVE). It is shown that the normalization constraint plays an important role in keeping the higher cluster terms small. The resulting LOCVE calculation for the ground state energy of liquid ^{3}He is compared with the available experimental data and the prediction from different theoretical techniques.

PACS. 61.20.Gy Theory and models of liquid structure – 61.20.Ne Structure of simple liquids – 67.55.-s Normal phase of liquid ^{3}He

1 Introduction

Liquid helium 3 is a very exceptional system. It behave's like a normal liquid and obeys the Landau Fermi liquid theory when the temperature is sufficiently low i.e. $T_c = 0.0026$ K $< T < 0.16$ K, while it becomes superfluid below the critical temperature T_c. This shows the important effects of many-body correlations and the interatomic interaction which has a strong repulsive hard-core. In this paper we deal only with the normal-liquid phase of ^{3}He since we have its experimental equation of state [2].

There are three proposes in studying such a system: (i) to obtain the normal liquid helium-3 properties and compare the results with experiment, (ii) to test different many-body methods against each other and (iii) to investigate the validity of the LOCV techniques.

Because of the simplicity of the interaction, most of the available many-body methods have been applied to liquid ^{3}He. Therefore, this system can be considered as a good testing ground for comparison of different many-body techniques.

In a series of papers [3,4], the lowest order constrained variational (LOCV) method was developed for calculating the properties of homogeneous nuclear fluids with realistic nucleon-nucleon interactions [5]. In 1998, this approach was further generalized to include more sophisticated interactions such as the UV_{14} [5], the AV_{14} [6] and the new argonne AV_{18} [7] as well as the Reid [5] and Δ-Reid [4,8] potentials. For a wide range of models our LOCV calculations agree well with the results of fermion hypernetted chain (FHNC) calculations. The LOCV calculations have been performed for a number of central potentials and are in agreement with the essentially exact numerical solutions obtained by Monte Carlo techniques [3,4]. Despite this agreement for model problems, there has been some dispute about the convergence of LOCV results in calculations, which employ realistic nucleon-nucleon interactions that are strongly spin-dependent and which, in particular, contain a sizeable tensor force. This argument was tested by calculating the energy of the three-body cluster contribution in nuclear matter, and the normalization integral $\langle\psi \mid \psi\rangle$, both at zero and finite temperatures [9]. It was shown that $\langle\psi \mid \psi\rangle$ is normalized within one percent, and that the three-body cluster energy is less than 1 MeV for $k_f \leq 1.6$ fm^{-1}.

Our LOCV calculation is a fully self-consistent technique that is capable of dealing with the well-defined phenomenological potentials such as the Δ-Reid (the modified Reid potential with an allowance for $\Delta(1234)$ degrees of freedom, see references [4,8]) potential. The Δ state, being the most important configuration which modifies the nuclear force, might be the key to the understanding of three-body forces [10]. The results suggest that the LOCV method reasonably describes the properties of nucleonic-matter at both zero and finite temperatures [4,10].

Furthermore, our calculations at zero temperature with the UV_{14} and AV_{18} potentials [10] shows a good agreement with more sophisticated calculation such

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as the variational fermion hypernetted chain method (FHNC) [6,11].

The LOCV method has been also developed for calculating the various properties of homogeneous nuclear fluids, such as hot and frozen neutron, nuclear and β-stable matter with realistic nucleon-nucleon interactions [10]. In these works the liquid-gas phase transition and corresponding critical temperature were found.

Recently, we applied LOCV formalism to the homogeneous electron fluid at finite temperature [12] and found satisfactory results.

However, liquid ^{3}He is a much more dense system than both nuclear matter and the electron fluid [12]. In other words ^{3}He, atoms are approximately three times more compressed than the nucleons in nuclear matter. So in general, the conventional many-body theories such as the Brueckner-Bethe calculation do not work. We also expect that the cluster expansion series does not converge as it does for nuclear matter, especially as we increase the density.

Given the above arguments, in this work we shall attempt to calculate the properties of uniform liquid helium-3 by using different ^{3}He–^{3}He potentials, and we shall investigate the convergence of the cluster expansion.

Various many-body techniques have been applied to ^{3}He fluid: Variational, Diffusion and Euler Monte Carlo (VMC, DMC, EMC) [13], variational Fermi-Hypernetted-Chain (FHNC) [14,15] and Density Functional Approximation (DFA) [16]. We also compare our results with these techniques and the available experimental data [2] to find out the accuracy of LOCV calculations with pure central forces.

The rest of this paper is planned as follows: in Section 2 we present the uniform ^{3}He fluid Hamiltonian with a short description of the lowest order constrained variational method, and the evaluation of its ground state energy. The three-body cluster energy is derived in Section 3. Finally, in Section 4 we present the results and further discussions.

2 The LOCV formalism

The total Hamiltonian of the liquid ^{3}He is usually written as [1]:

$$\mathcal{H}_{^3\mathrm{He}} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2}\sum_{i\neq j}^{N} v(ij), \tag{1}$$

where $v(ij)$ is the interatomic potential. In this work we consider Lennard-Jones and Aziz potentials [17].

In the LOCV method, we use an ideal Fermi gas type wave function for the single particle states and we use variational techniques to find the wave function of interacting system [3,4,11], i.e.

$$\psi = \mathcal{F}\varPhi, \tag{2}$$

and (where $\mathcal{S}$ is a symmetrizing operator),

$$\mathcal{F} = \mathcal{S}\prod_{i>j} f(ij). \tag{3}$$

In general, the Jastrow correlation functions $f(ij)$ are operators. In the case of ^{3}He fluid however because of the simplicity of interatomic interaction we assume them to depend only on the relative distance of two particles.

The ^{3}He fluid energy is written as [3,4,11],

$$E = T_F + E_{MB}[f]. \tag{4}$$

T_F is simply the Fermi gas kinetic energy, and is defined by

$$T_F = (\varOmega\rho)^{-1}\sum_{k,\sigma\tau} \frac{\hbar^2 k^2}{2m}\theta(k_F - k). \tag{5}$$

The fluid density ρ will fix the Fermi-momentum $k_F(= (3\pi^2\rho)^{\frac{1}{3}})$.

The many-body energy term $E_{MB}[f]$ is calculated by constructing a cluster expansion for the expectation value of our Hamiltonian $\mathcal{H}_{^3\mathrm{He}}$ of equation (1). Then we only keep the first two terms in a cluster expansion of the energy functional [18] such as:

$$E[f] = \frac{1}{N}\frac{\langle\varPsi|H|\varPsi\rangle}{\langle\varPsi|\varPsi\rangle} = T_F + E_{MB} = T_F + E_2 + E_3 + \ldots \tag{6}$$

The two-body energy term is defined as

$$E_2 = (2N)^{-1}\sum_{ij}\langle ij|\mathcal{V}|ij\rangle_a \tag{7}$$

where

$$\mathcal{V}(12) = -\frac{\hbar^2}{2m}[f(12),[\nabla_{12}^2, f(12)] + f(12)V(12)f(12), \tag{8}$$

and the two-body antisymmetrized matrix element $\langle ij|\mathcal{V}|ij\rangle_a$ are taken with respect to the single-particle functions composing $\varPhi$, i.e. plane-waves.

In the LOCV formalism, E_{MB} is approximated by E_2, and one hopes that the normalization constraint makes the cluster expansion converges very rapidly and bring the many-body effect into the E_2 term.

For the ^{3}He fluid, because of the choice of correlation functions, the two-body effective interaction in equation (8) is reduced to the following equation:

$$\mathcal{V}(12) = \frac{\hbar^2}{m}(\nabla f(12))^2 + f(12)^2 v(12). \tag{9}$$

Now, by using plane waves as the single-particle states, equation (7) reduces to:

$$E_2 = \frac{1}{2}\rho\int \mathcal{G}_F(r)\mathcal{V}(r)d\mathbf{r}, \tag{10}$$

where

$$\mathcal{G}_F(r) = [1 - \frac{1}{2}l^2(k_F r)] \tag{11}$$

and

$$l(x) = 3\frac{J_1(x)}{x}. \tag{12}$$

$J_l(x)$ are the familiar spherical Bessel functions.

The normalization constraint [19] is given by:

$$\rho\int(\mathcal{G}_2(r_{12})-1)d\mathbf{r_{12}}=-1, \tag{13}$$

where [18]

$$\mathcal{G}_2(r_{12})=f^2(r_{12})\sum_{n=2}^{N}[\varDelta\mathcal{G}(r_{12})]_n. \tag{14}$$

The first two terms that we intend to use later are:

$$[\varDelta\mathcal{G}_2(r_{12})]_2=\mathcal{G}_F(r_{12}),$$

$$\begin{aligned}&[\varDelta\mathcal{G}_2(r_{12})]_3=\\&-\rho\int d\mathbf{r_{13}}h(r_{13})[l^2(k_Fr_{23})-l(k_Fr_{12})l(k_Fr_{23})l(k_Fr_{13})]\\&\qquad+\rho\int d\mathbf{r_{13}}h(r_{13})h(r_{23})\mathcal{G}_{3F}(r_{12},r_{23},r_{13}),\end{aligned}$$

$$\begin{aligned}&\mathcal{G}_{3F}(r_{12},r_{23},r_{13})=1-\frac{1}{2}\left[l^2(k_Fr_{12})\right.\\&\left.+l^2(k_Fr_{23})+l^2(k_Fr_{13})+\frac{1}{2}l(k_Fr_{12})l(k_Fr_{23})l(k_Fr_{13})\right].\end{aligned}$$

By keeping only $n=2$ terms in the two-body distribution function, the normalization constraint of equation (13) can be written as,

$$\rho\int(\mathcal{G}_F(r)^{-1}-f(r)^2)\mathcal{G}_F(r)d\mathbf{r}=-1, \tag{15}$$

or

$$\langle\psi|\psi\rangle=\rho\int\mathcal{G}_F(r)f^2(r)d\mathbf{r}=1, \tag{16}$$

which is the constraint used in our previous works.

Note that $\xi=[\langle\psi|\psi\rangle-1]$ plays the role of a smallness parameter in the cluster expansion. The above constraint introduces another parameter in our formalism, i.e. the Lagrange multiplier λ. By using the Euler-Lagrange equation, we minimize the functional $\mathcal{L}(r,f,f')=r^2\{E_2+\lambda\langle\psi|\psi\rangle\}[f]$ with respect to $f(r)$ and we choose λ such that the above normalization constraint is satisfied, i.e.

$$\frac{\partial\mathcal{L}}{\partial f(r)}-\frac{\partial}{\partial r}\frac{\partial\mathcal{L}}{\partial f'(r)}=0. \tag{17}$$

This leads to the following differential equation:

$$g''(r)-\left[\frac{A''(r)}{A(r)}+\frac{m}{\hbar^2}(v(r)-\lambda)\right]g(r)=0, \tag{18}$$

where

$$g(r)=A(r)f(r) \tag{19}$$

and

$$A(r)^2=r^2\mathcal{G}_F(r). \tag{20}$$

Therefore the constraint is incorporated by solving the above Euler-Lagrange equation (18) out to certain distances where the logarithmic derivative of correlation function $f(r)$ matches that of $\mathcal{G}_F^{-\frac{1}{2}}$, and then we set the correlation function equal to $\mathcal{G}_F^{-\frac{1}{2}}$ (note that $\mathcal{G}_F^{-\frac{1}{2}}$ satisfies the boundary condition $f(r\to\infty)\to1$).

3 Three-body cluster term

In order to test the accuracy of the LOCV method, we use the calculated two-body correlation function $f(r)$ and the two-body effective interaction $\mathcal{V}(r)$ to evaluate the three-body cluster energy [18]:

$$E_3=[E_{3(2)}]+E_{3(3)}+E_{4(2)}=[E_{3h}+E_{3hh}]+E_{3t}+E_{4h}, \tag{21}$$

$$\begin{aligned}E_{3h}=\frac{1}{N}\sum_{ijk}[&\langle ijk\mid h(r_{13})\mathcal{V}(r_{12})\mid ijk\rangle_a\\&+\langle ik\mid h(r_{13})\mid ik\rangle_a\langle ij\mid\mathcal{V}(r_{12})\mid ij\rangle_a],\end{aligned} \tag{22}$$

$$E_{3hh}=\frac{1}{2N}\sum_{ijk}\langle ijk\mid h(r_{13})\mathcal{V}(r_{12})h(r_{23})\mid ijk\rangle_a, \tag{23}$$

$$E_{3t}=\frac{1}{2N}\sum_{ijk}\langle ijk\mid\frac{\hbar^2}{2m}f^2(r_{12})\nabla_2h(r_{12})\cdot\nabla_2h(r_{23})\mid ijk\rangle_a, \tag{24}$$

$$E_{4h}=\frac{1}{N}\sum_{ijkl}\langle ik\mid h(r_{13})\mid jl\rangle_a\langle jl\mid\mathcal{V}(r_{12})\mid ik\rangle_a. \tag{25}$$

Note that the last term in the above equation is a special portion of the four-body terms which are proportional to the smallness parameter ξ, like the three-body cluster terms. After some straightforward calculations, we can write equations (22) to (25) as follows:

$$\begin{aligned}E_{3h}=\frac{\rho^2}{2}\int d\mathbf{r_{12}}\int d\mathbf{r_{13}}&h(r_{13})l(k_Fr_{23})\mathcal{V}(r_{12})[-l(k_Fr_{23})\\&+\frac{1}{2}l(k_Fr_{13})l(k_Fr_{12})],\end{aligned} \tag{26}$$

$$\begin{aligned}&E_{3hh}=\frac{\rho^2}{2}\int d\mathbf{r_{12}}\int d\mathbf{r_{13}}h(r_{13})h(r_{23})\mathcal{V}(r_{12})\\&[1-\frac{1}{2}l^2(k_Fr_{12})-l^2(k_Fr_{13})+\frac{1}{2}l(k_Fr_{12})l(k_Fr_{23})l(k_Fr_{13})],\end{aligned} \tag{27}$$

$$\begin{aligned}&E_{3t}=\\&\frac{\rho^2}{2}\int d\mathbf{r_{12}}\int d\mathbf{r_{13}}(h(r_{13})+1)h'(r_{12})h'(r_{23})\left(\frac{\mathbf{r_{12}}\cdot\mathbf{r_{23}}}{r_{12}r_{23}}\right)\\&\left[1-\frac{1}{2}l^2(k_Fr_{12})-l^2(k_Fr_{13})+\frac{1}{2}l(k_Fr_{12})l(k_Fr_{23})l(k_Fr_{13})\right],\end{aligned} \tag{28}$$

$$\begin{aligned}&E_{4h}=\\&\frac{\rho^3}{8}\int d\mathbf{r_{12}}\int d\mathbf{r_{13}}\int d\mathbf{r_{14}}h(r_{34})l(k_Fr_{13})l(k_Fr_{24})\mathcal{V}(r_{12})\\&\left[l(k_Fr_{13})l(k_Fr_{24})-\frac{1}{4}l(k_Fr_{14})l(k_Fr_{23})\right],\end{aligned} \tag{29}$$

where

$$h(ij)=f^2(ij)-1. \tag{30}$$

Table 1. Results of the LOCV calculation for the ground state energy of liquid ^{3}He as afunction of density. The FHNC results of Krotsscheck [15] and Owen [14] are given for comparison (μ is the FHNC variational parameter [15]). The last column are the corresponding experimental values [2].

ρ(A^{-3})	μ(FHNC)	FHNC(K)[15]	FHNC(K)[19]	LOCV(K)	EXP(K)
0.0100	0.775	–0.906	-0.83	–1.55[–1.25]	–
0.0108	0.780	–0.964	-	–1.86[–1.31]	–
0.0116	0.780	–1.027	-	–1.74[–1.29]	–
0.0124	0.785	–1.058	-	–1.70[–1.11]	–
0.0132	0.785	–1.067	-	–1.55[–0.80]	–
0.0140	0.785	–1.055	–0.75	–1.26[0.30]	–
0.0148	0.785	–1.020	-	–0.85[0.41]	–
0.0156	0.790	–0.963	-	–0.77[1.35]	–
0.0164	0.790	–0.879	-	–0.77[2.57]	–2.52
0.0172	0.795	–0.781	-	–0.69[4.08]	–2.49
0.0180	0.795	–0.640	–0.11	+3.25[5.91]	–2.43

Next we simply add the contribution of the three-body cluster energy, E_3, to the two-body energy E_2. It is clear that the sum $E_2 + E_3$ should not be considered as the variational energy, since we have to vary $E_2 + E_3 + \ldots$ simultaneously to find the upper bound to the true ground state energy. In other words, E_3 is just an estimate to the three-body cluster energy therefore So $E_2 + E_3$ should not be considered as the upper bound to the true energy. however, if we find that E_3 is very small compared to E_2, i.e. the cluster expansion converges very rapidly, then we can conclude that $T_F + E_2$ is a good approximation for the upper bound ground state energy of liquid ^{3}He.

4 Results and discussion

In Table 1 we present the result of the LOCV calculation for the ground state energy of helium 3 liquid for different densities. The values in the brackets are the same calculation but with the Aziz potential [17]. It is seen that these energies are rather poor with respect to the corresponding experimental saturation value of –2.52 K at $\rho = 0.0164$ A^{-3} [2]. There is not much difference between Aziz and Lennard-Jones potentials at low densities. The FHNC results of Krotschrck [15] and Owen [14] are also given for comparison. The LOCV energies are very similar to those of FHNC, especially at low densities.

In Figure 1 the LOCV correlation functions are shown for two different densities, i.e. $\rho = 0.01$ and 0.018 A^{-3}. The FHNC correlation functions [15] are also plotted for comparison. It is seen that the LOCV correlation functions have much more density dependence than the FHNC calculations. In general, because we have a high density system with strong repulsive cores, we expect that the correlation functions show a strong density dependence such as those of LOCV, rather than the weak one produced by FHNC calculations.

In order to see the effect of normalization constraint, in Figure 2 we have plotted the ratio of three-body to two-body cluster energies versus χ (the convergence parameter at $\rho = 0.015$ A^{-3}). It is seen that the ratios are small especially near $\chi = 0$, and we can conclude that the normalization constraint forces the higher cluster terms to become small. One should notice that near $\chi = 0.25$, the two-body energy becomes zero at $\rho = 0.015$ A^{-3}. Therefore the ratios show a large peak.

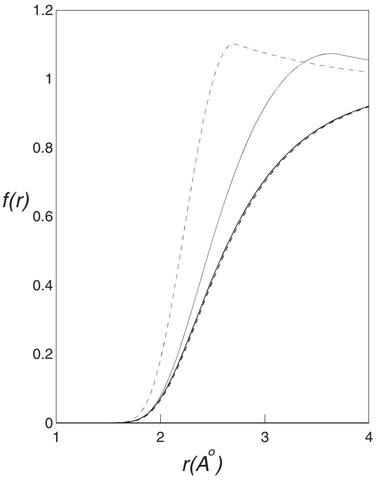

Fig. 1. Comparison of the LOCV correlation functions at two different density, $\rho = 0.01$ (full curve) and 0.018 fm^{-3} (dashed curve). The FHNC results of Krotscheck [15] are also given for $\mu = 0.775$ (heavy full) and 0.795 (heavy dashed) for both pf the above densities.

In order to improve our LOCV result presented in Table 1, we have extended our two-body distribution function to include three-body correlation ($n = 3$) in equation (14). We have used the new distribution function in the normalization constraint (Eq. (13)). With this change, the Euler-Lagrange differential equation (18) becomes an integral-differential equation in terms of $f(r_{12})$. We have solved this equation iteratively with our constraint until the energy is saturated, i.e until the continuation of

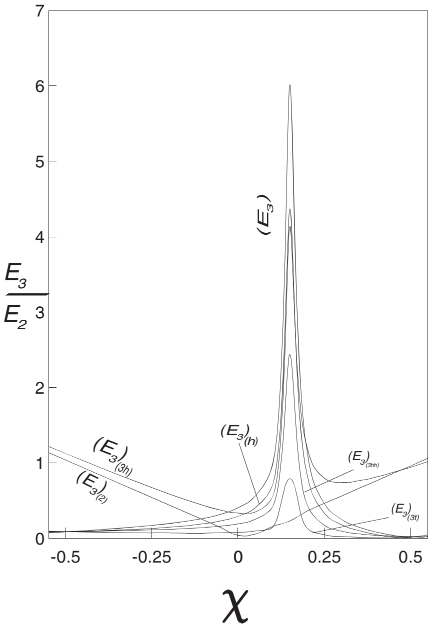

Fig. 2. Ratio of E_3/E_2 versus χ.

iteration does not change the energy at each density. The result of LOCV calculation with an extended constraint (LOCVE) for the ground state of liquid ^{3}He is plotted in Figure 3 (full curve). The dashed curve is the LOCVE with contributions from the three-body cluster energy. However, as we have pointed out before, this can not be considered as the variational energy. The heavy-full, dashed and dotted curves are the experimental [2], diffusion (DMC) and variational (VMC) Monte Carlo [13] calculations respectively. There is overall agreement between them at low densities $\rho < 0.018$ A^{-3}. However, beyond this density the LOCVE result shows much more density dependence than the experimental data, DMC and VMC calculations.

Finally in Figure 4 we compare the LOCV and LOCVE healing distances. It is shown that the correlation functions have longer range in the case of LOCVE than LOCV.

In conclusion, we have developed the LOCVE formalism to calculate the ground state energy of liquid ^{3}He. It is shown that while the three-body cluster energy is small, the three-body correction to the normalization constraint plays an important role in the ground state energy calculation of liquid ^{3}He. Therefore one can conclude that for high density systems, the correction to the two-body distribution is much more important than the same correction for the energy calculations. On the other hand, the normalization constraint plays an important role in keeping the higher order cluster terms small in the cluster expansion series. It was also shown that the LOCVE gives the same result as the more sophisticated methods such as DMC and VMC.

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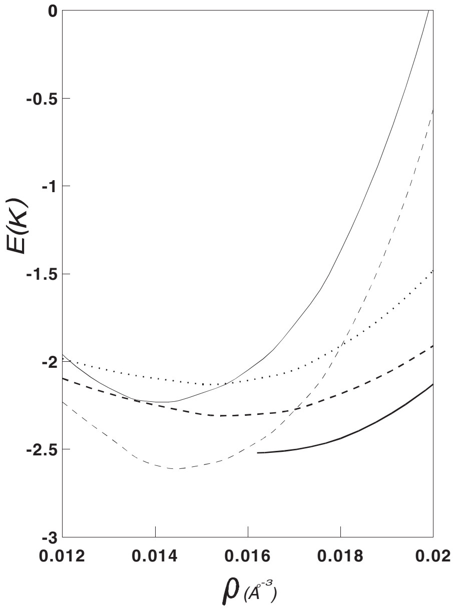

Fig. 3. Comparison of the extended LOCV calculation for the ground state energy of liquid helium 3, with (dashed curve) and without (full curve) the contribution from the three-body cluster energy E_3. Heavy full, dash and dotted curves are the experimental, DMC and VMC results, respectively.

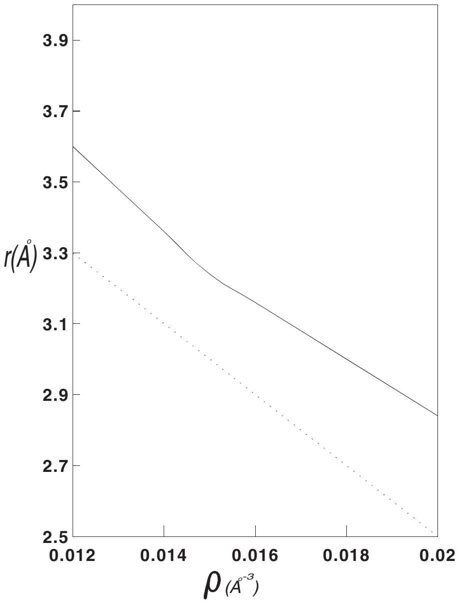

Fig. 4. Healing distances of the two-body correlation function against density with full (LOCVE) and dotted (LOCV) curves.

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