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LOCV calculation for the uniform electron fluid at finite temperature

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Abstract. The free energy of the homogeneous electron fluid at finite temperature is obtained using the lowest order constrained variational (LOCV) method. In order to test the convergence of cluster expansion series the three-body cluster terms are calculated with the LOCV correlation functions. The results agree reasonably with those of Monte Carlo, coupled-cluster, perturbational expansion etc, techniques at zero temperature. The flashing and critical temperatures as well as the critical exponent are found to be about 0.6, 1.3 eV and 0.384 respectively. A similar liquid-gas phase transition to that of nuclear matter and liquid He^3 is observed.

PACS. 64.70.Fx Liquid-vapor transitions – 71.10.-w Theories and models of many-electron systems – 71.10.Ca Electron gas, Fermi gas – 64.60.Fr Equilibrium properties near critical points, critical exponents

1 Introduction

The uniform electron fluid consists of N electrons embedded in N positively charged ion background at the thermodynamic limit, such that their densities $\rho = \frac{N}{\Omega}$ (Ω is the volume) are constant [1]. It is possible to distinguish three different regions of interest in terms of r_s, the Wigner-Seitz radius in units of Bohr radius, for this system: the weak $r_s \leq 1$, intermediate $1 \leq r_s \leq 10$ and strong $r_s \geq 10$ coulomb coupling regions. The weak-coupling and the intermediate-coupling have been extensively studied and some accurate results have been obtained.

There are two points in studying such a ideal system: (i) To obtain the metals properties. (ii) To test different many-body methods against each other.

Obviously the homogeneous electron fluid is not very good model for the real physical systems such as metals. But, at least, it could be considered as an input data for the local density approximation calculations.

Because of the simplicity of the interaction, most of the available many-body methods have been mainly applied to the uniform electron fluid at zero temperature. So this system can be considered as a good testing ground for comparison of different many-body techniques. On the other hand, some of the many-body methods have been only designed and applied to the problems which involve short range interactions. Then it would be interesting to apply these techniques to the uniform electron fluid, with its long-range coulomb interaction [2], to find out about the accuracy and performance of these methods.

In a series of papers the lowest order constrained variational (LOCV) method was developed [3,4] 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} [7], 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 where these have performed and for a number of central potentials, there is agreement with the essentially exact numerical solutions obtained by Monte Carlo technique [3,4]. Despite this agreement for model problems, there has been some dispute about the convergence of LOCV results in calculations, employing realistic nucleon-nucleon interactions which 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 the three-body cluster energy is less than 1 MeV for $k_f \leq 1.6\ \text{fm}^{-1}$.

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Our LOCV calculation is a fully self-consistent technique and is capable of dealing with the well-defined phenomenological potentials such as the Δ-Reid (the modified Reid potential with an allowance of $\Delta(1234)$ degree of freedom, see references [4,8]) potential. The Δ state, being the most important configuration that 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 nucleonic-matter properties at zero and finite temperatures [4,10].

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

With respect to the above arguments, in this work we shall attempt to calculate the properties of uniform electron fluid at finite temperature by using the long-range coulomb potential and investigate the behavior of its equation of state with the temperatures and densities.

Various many-body techniques have been applied to the homogeneous electron fluid: perturbational expansion (PE) [12], variational and diffusion Monte Carlo (VMC, DMC) [13], variational Fermi-hypernetted-chain (FHNC) [2,14], coupled-cluster expansion (CCE) [15], density functional approximation (DFA) [16], random phase approximation (RPA) [17] and numerical many-body perturbation expansion (NPE) [18] methods. So we can compare our results with these techniques to find out about the accuracy of LOCV calculations with long-range forces.

So the paper is planned as follows: In Section 2 we present the uniform electron fluid Hamiltonian. A short description of the lowest order constrained variational method and the evaluation of internal energy of uniform electron fluid with LOCV method is given in Section 3. The three-body cluster energy is derived in Section 4. Finally, in Section 5 we calculate the electron gas entropy and we present the results and discussions.

2 The uniform electron fluid Hamiltonian

The total Hamiltonian of uniform electron fluid with positive background is usually written as [1]:

$$H = H_{el} + H_b + H_{el-b} \tag{1}$$

where H_{el}, H_b and H_{el-b} are the electron, positive-background and electron-positive-background Hamiltonian respectively. This Hamiltonian can be reduced to [1],

$$H = -\frac{1}{2} e^2 N^2 \Omega^{-1} 4\pi \mu^{-2} + H_{el} \tag{2}$$

in which

$$\begin{aligned} H_{el} &= \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2} e^2 \sum_{i\neq j}^{N} \frac{\mathrm{e}^{-\mu|\mathbf{r_i}-\mathbf{r_j}|}}{|\mathbf{r_i}-\mathbf{r_j}|} \\ &= \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i\neq j}^{N} V(ij). \end{aligned} \tag{3}$$

The exponential factor and the parameter μ are introduced in this Hamiltonian to make the calculations finite. Then after performing many-body calculations, usually the parameter μ, sets to zero, if one intends to have only the coulomb interaction.

3 The LOCV formalism

In the LOCV method, we use an ideal Fermi gas type wave function for the single particle states and variational techniques, to find the wave function of interacting system [3,4,11] at finite temperature $\mathcal{T}$ *i.e.*,

$$\psi = \mathcal{F}_{\mathcal{T}} \Phi^{\mathcal{T}} \tag{4}$$

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

$$\mathcal{F}_{\mathcal{T}} = \mathcal{S} \prod_{i>j} f(ij). \tag{5}$$

In general, the Jastrow correlation functions $f(ij)$ are operators. But in case of uniform electron fluid, because of the simplicity of coulomb interaction, we assume them to have the following form:

$$\begin{aligned} f(r) &= 1 - \exp(-ur) + A_0 \exp\left[-\alpha(r-r_c)^2\right] \\ &= 1 + C(r) \end{aligned} \tag{6}$$

where $r_c = \frac{1}{u}$ and the parameters u, A_0 and α are calculated variationally.

The electron fluid internal energy is written as [3,4,11],

$$E_{in} = T_F + E_{MB}[f]. \tag{7}$$

T_F is simply the Fermi gas kinetic energy and it is defined as

$$T_F = (\Omega\rho)^{-1} \sum_{k,\sigma\tau} \frac{\hbar^2 k^2}{2m} n(k). \tag{8}$$

The fluid density ρ will fix the chemical potential μ,

$$\rho = \Omega^{-1} \sum_{\sigma,\tau,k} n(k) \tag{9}$$

where

$$n(k) = \left[\exp((\varepsilon^*(k) - \mu)\beta) + 1\right]^{-1}. \tag{10}$$

$n(k)$ is the Fermi-Dirac distribution function, $\beta = \frac{1}{k_B \mathcal{T}}$ and k_B is the Boltzmann factor (we assume $k_B = 1$, so the temperature is in eV units). The single particle energy is approximately written in terms of effective mass *i.e.* $\varepsilon^*(k) = \frac{\hbar^2 k^2}{2m^*}$ and the effective mass, m^*, is determined variationally (m^* varies between zero and one, see references [6] and [11] for detail).

The many-body energy term $E_{MB}[f]$ is calculated by constructing a cluster expansion for the expectation value of our Hamiltonian H_{el} of equation (3). Then, we keep only the first two terms in a cluster expansion of the energy functional [19]:

$$E[f] = \frac{1}{N}\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = T_F + E_{MB} = T_F + E_2 + E_3 + \ldots \tag{11}$$

The two-body energy term is defined as,

$$E_2 = (2N)^{-1}\sum_{ij}\langle ij|\mathcal{V}|ij\rangle_a \tag{12}$$

where

$$\mathcal{V}(12) = -\frac{\hbar^2}{2m}\left[f(12),\left[\nabla_{12}^2, f(12)\right]\right] + f(12)V(12)f(12) \tag{13}$$

and the two-body antisymmetrized matrix elements $\langle ij|\mathcal{V}|ij\rangle_a$ are calculated by using plane-waves.

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

For the electron fluid, because of the choice of correlation functions, the two-body effective interaction, equation (13) is reduced to the following equation:

$$\begin{aligned}\mathcal{V}(12) &= \frac{\hbar^2}{m}\left[\nabla f(12)\right]^2 + f(12)^2 V(12)\\ &= \frac{\hbar^2}{m}[\nabla C(r)]^2 + C(r)\left[2 + C(r)\right]V(r) + V(r).\end{aligned} \tag{14}$$

Now, by using plane waves as the single-particle states, equation (12) reduces to:

$$E_2 = \frac{1}{2}\rho\int g_F(r)\mathcal{V}(r)\mathrm{d}\mathbf{r} \tag{15}$$

where

$$g_F(r) = \left[1 - \frac{1}{2}(\frac{\gamma(r)}{\rho})^2\right] = 1 + C_F(r) \tag{16}$$

with

$$\gamma(r) = \frac{2}{(2\pi)^3}\int n(k)J_0(kr)\,\mathrm{d}\mathbf{k}. \tag{17}$$

$J_J(x)$ are the familiar spherical Bessel functions. Finally the two-body cluster energy is written as:

$$\begin{aligned}E_2 = \frac{1}{2}\rho\Bigg[\int V(r)\mathrm{d}\mathbf{r} + \int C_F(r)V(r)\mathrm{d}\mathbf{r} + \int\Bigg[(1 + C_F(r))\\ \times\left[\frac{\hbar^2}{m}(\nabla C(r))^2 + C(r)(2 + C(r))V(r)\right]\mathrm{d}\mathbf{r}\Bigg]\Bigg].\end{aligned} \tag{18}$$

The first integral in E_2 will be canceled exactly with the first term in the total Hamiltonian of equation (2) [1]. While the second term, the Hartree-Fock energy, and the third term can be considered as the correlation energy.

The normalization constraint can also be written as following:

$$\langle\psi|\psi\rangle = \rho\int(1 + C_F(r))(1 + C(r))^2\mathrm{d}\mathbf{r} = 1. \tag{19}$$

Note that $\xi = [\langle\psi|\psi\rangle - 1]$ plays the role of smallness parameter in the cluster expansion. The above constraint introduces another parameter in our formalism *i.e.* the Lagrange multiplier λ. So at zero (finite) temperature we minimize the functional $\{E_2 + \lambda\langle\psi|\psi\rangle\}[f]$ (free energy, see Sect. 5) respect to the parameters u, A_0, α (including m^* at finite temperature) and we chose λ such that the above normalization constraint is satisfied.

4 Three-body cluster term

In order to test the accuracy of 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 [19] *i.e.*:

$$\begin{aligned}E_3 = \frac{1}{N}\sum_{ijk}\langle ijk \mid h(r_{13})\mathcal{V}(r_{12}) \mid kij - ijk\rangle\\ + \frac{1}{2N}\sum_{ijk}\langle ijk \mid h(r_{13})\mathcal{V}(r_{12})h(r_{23}) \mid ijk\rangle_a\\ + \frac{1}{2N}\sum_{ijk}\left\langle ijk\left|\frac{\hbar^2}{2m}f^2(r_{12})\nabla_2 h(r_{12})\cdot\nabla_2 h(r_{23})\right|ijk\right\rangle_a\\ + \frac{1}{N}\sum_{ijkl}\langle ik \mid h(r_{13}) \mid jl\rangle_a\langle jl \mid \mathcal{V}(r_{12}) \mid ik\rangle_a\cdot\end{aligned} \tag{20}$$

Note that the last term in above equation is a special portion of the four-body terms which is proportional to the smallness parameter ξ, like the three-body cluster terms. Then after doing some straightforward operation, we can write equation (20) as following:

$$\begin{aligned}E_3 = \int\mathrm{d}\mathbf{r_{12}}\int\mathrm{d}\mathbf{r_{13}}\Bigg\{\Bigg\{h(r_{13})\Bigg[\frac{1}{\nu}\gamma(r_{23})(\gamma(r_{23})\\ + \frac{1}{\nu}\gamma(r_{13})\gamma(r_{12})) + \frac{1}{2}h(r_{23})\Bigg[1 - 2\gamma^2(r_{23}) - \frac{1}{\nu}\gamma^2(r_{12})\\ + \frac{2}{\nu^2}\gamma(r_{12})\gamma(r_{23})\gamma(r_{13})\Bigg]\Bigg] + \frac{1}{2\nu^2}\int\mathrm{d}\mathbf{r_{14}}\gamma(r_{13})\gamma(r_{24})\\ \times\left[h(r_{24})\gamma(r_{13})\gamma(r_{24}) - \frac{1}{\nu}h(r_{34})\gamma(r_{14})\gamma(r_{23})\right]\Bigg\}\mathcal{V}(r_{12})\\ + \frac{1}{2}(h(r_{13}) + 1)h'(r_{12})h'(r_{23})\left(\frac{\mathbf{r_{12}}\cdot\mathbf{r_{23}}}{r_{12}r_{23}}\right)\\ \times\left[1 - 2\gamma^2(r_{23}) - \frac{1}{\nu}\gamma^2(r_{12}) + \frac{2}{\nu^2}\gamma(r_{12})\gamma(r_{23})\gamma(r_{13})\right]\Bigg\}\end{aligned} \tag{21}$$

where

$$h(ij) = f^2(ij) - 1 = C(ij)(2 + C(ij)) \tag{22}$$

and for the electron fluid the degeneracy parameter $\nu = 2$. Then we can 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 $E_2 + E_3$ (at zero temperature) 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, *i.e.* E_3 is just an estimate to the three-body cluster energy. So $E_2 + E_3$ should not be considered as the upper bound to the true energy. But if we find that E_3 is very small respect to E_2 *i.e.* the cluster expansion is converges very rapidly, we can conclude that $T_F + E_2$ is a good approximation for the electron gas upper bound ground state energy. However, as it will be mentioned in the next section, the variation of $E_2 + E_3$ gives the same contribution as the one we get by varying E_2 and then calculating E_3 as a correction.

5 Results and discussion

The total free energy $F(\rho, T, m^*)$ is computed by minimizing $T_F + E_2 - \mathcal{T}S$ with respect to the $C(r)$ and the spectrum parameter $m^*(\mathcal{T}, \rho)$ where S is the familiar Fermi-type isothermal entropy per particle [1] *i.e.*

$$S(\rho, \mathcal{T}, m^*) = -k_B(\Omega\rho)^{-1}\sum_{k,\sigma}[(1 - n(k))\ln(1 - n(k)) + n(k)\ln(n(k))]. \tag{23}$$

So $F(\rho, T, m^*)$ can now be differentiated to yield various quantities of interest such as pressure $P(\rho, \mathcal{T}, m^*)$ etc (note that m^* couples the internal energy and the entropy when we vary the free energy respect to all of the variational parameters, including m^*). It is found that for fixed ρ, α, u and A_0 the free energy is a smooth function of m^* (see Refs. [6] and [11]). This shows that the number of variational parameter we have considered in our LOCV calculation is enough.

We start by presenting our results for the frozen uniform electron fluid. In Figure 1, the dashed and full curves are our LOCV results without and with three-body terms (for $r_s = 4.17$, $E_{min} = -1.374$ eV with $\alpha = 0.511, A_0 = 0.101$ and $u = 2.013$). It is seen that they are not too different. The dotted curve represents the results of perturbation expansion (PE) [12] *i.e.*:

$$E = 13.6\left[2.21r_s^{-2} - 0.91r_s^{-1} + 0.0622\ln r_s - 0.0938 + 0.0184r_s\ln r_s - 0.020r_s + O\left(r_s^2\ln r_s, r_s^2\right)\right]. \tag{24}$$

The other available many-body methods, where quoted in Section 1, have also been shown by different marker style on this figure. For $r_s \leq 4$ our ground state energy results are very closed to PE (as we see later on, in this region, E_3 is less than 20% of E_2). The reason is obvious: for very high density, $r_s \to 0$, the LOCV correlation function goes to one for any separation and we get the same result as the perturbation expansion $(13.6[2.21r_s^{-2} - 0.91r_s^{-1}])$. On the other hand for $r_s \geq 4$ we get a similar density dependence behavior as those of FHNC, VMC etc. (our results are shifted about 1 eV upwards). So we can argue that the LOCV formalism even without the three-body energy is capable of dealing with long range forces such as coulomb interaction.

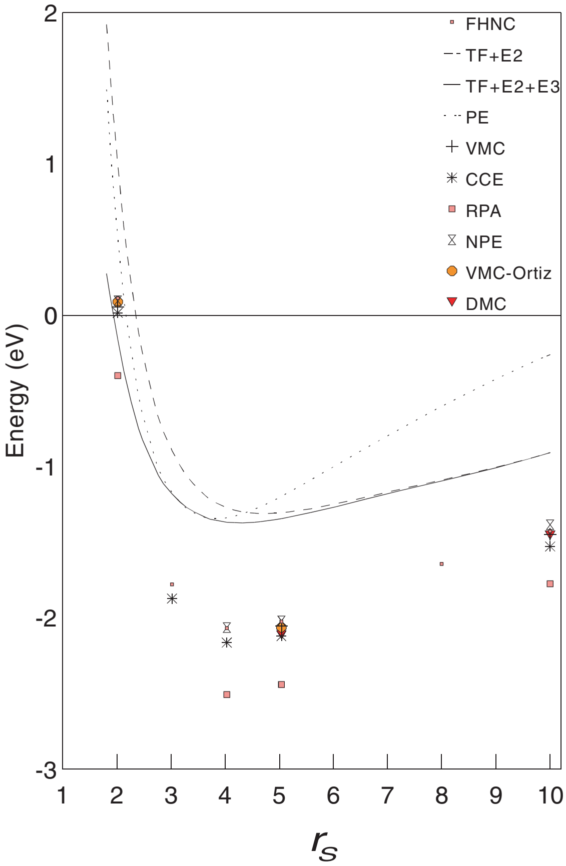

Fig. 1. Ground state energy (eV) of uniform electron fluid at zero temperature. Different curves and mark styles are according to the figure legend and text explanation.

The size of E_2 and E_3 are plotted in Figure 2. It is seen that for $r_s \geq 1.8$, E_3 is less than 2 eV (20% of E_2) and it vanishes for $r_s \geq 6$. It is very encouraging that E_3 is small. So we can argue that for this region (especially for $r_s \geq 1.8$) our LOCV method converges very rapidly and truncation of the cluster expansion after the two-body term is valid. As we pointed out before, we varied the whole two-body and three-body energies together and we found the same contribution for $E_2 + E_3$ as the one we obtained in Figure 2. But the individual contributions of E_2 and E_3 are different from the above LOCV case and the three-body term is no longer small respect to the two-body term, as one should expect. This again shows that the LOCV formalism with its constrained variational correlation functions makes the cluster expansion to converge rapidly.

Figure 3 shows the uniform electron fluid free energy with three-body cluster energy for different temperatures (eV) *versus* density (A^{-3}) (a typical value of the

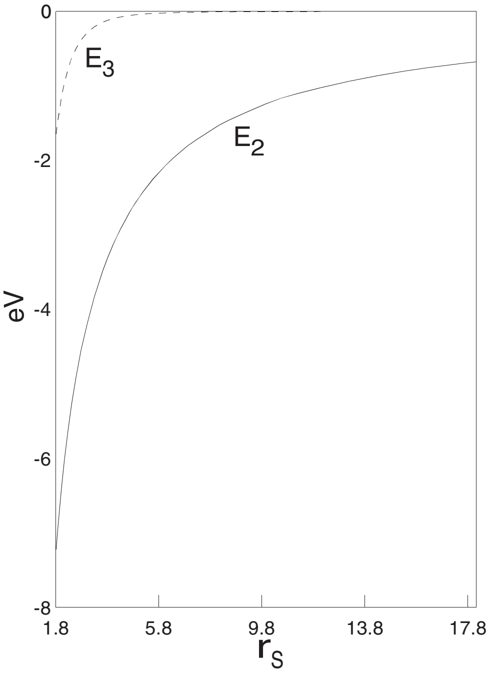

Fig. 2. The comparison of two-body and three-body cluster energy (eV) *versus* density (A^{-3}).

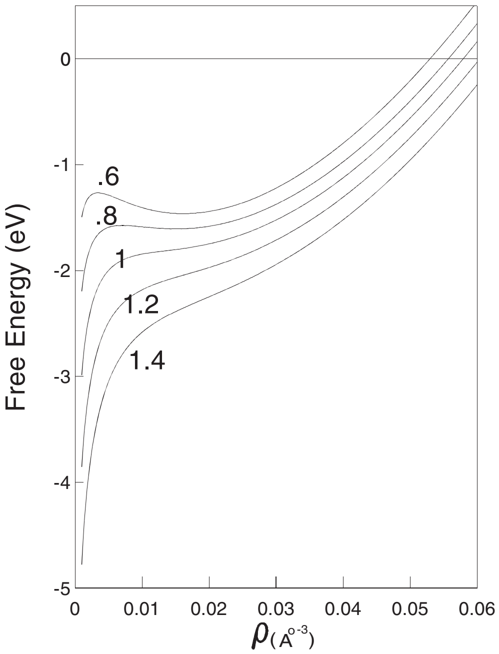

Fig. 3. The free energy of uniform electron fluid *versus* density (A^{-3}) at different temperatures (eV).

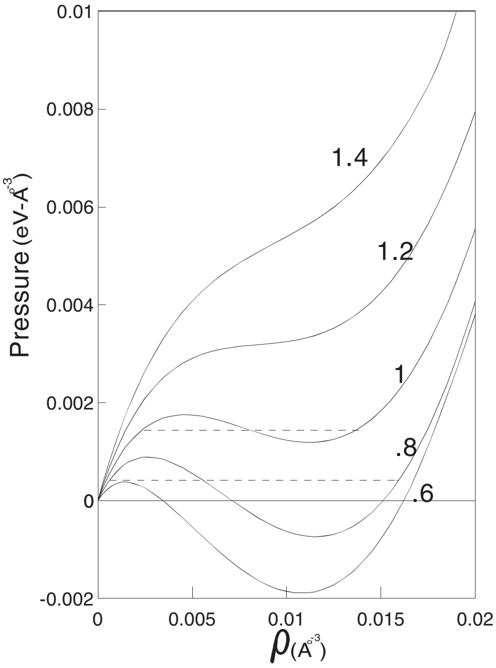

Fig. 4. As Figure 3 but for pressure ($\text{eV}\,A^{-3}$).

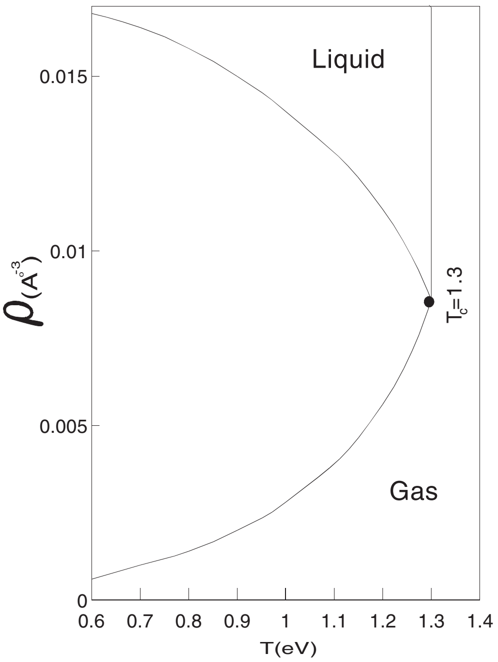

Fig. 5. The liquid-gas phase diagram.

variational parameters at $\mathcal{T} = 1$ eV and $\rho = 0.01\ A^{-3}$ with $F = -1.81$ eV are $\alpha = 0.312, A_0 = 0.081, u = 0.316$ and $m^* = 0.71$). Similar to our previous calculations [9–11], the free energy per particle decreases with increasing temperature at constant density. For temperatures greater than 1 eV the free energy is only increasing function of density.

The calculated pressure (P) ($\text{eV}\,A^{-3}$) is presented in Figure 4. The horizontal dashed lines show the gas-liquid phase transition. The thermodynamics conditions for the coexistence of two phases are:

$$\mu_{liquid}(\rho, \mathcal{T}) = \mu_{gas}(\rho, \mathcal{T}); P_{liquid}(\rho, \mathcal{T}) = P_{gas}(\rho, \mathcal{T}). \tag{25}$$

In order to find the exact value of critical temperature *i.e.* disappearance of liquid phase, in Figure 5 we plot the gas-phase diagram *i.e.* gas-liquid phase transition density *versus* temperature. It is seen that the critical temperature is about 1.3 eV. Near the critical temperature we can

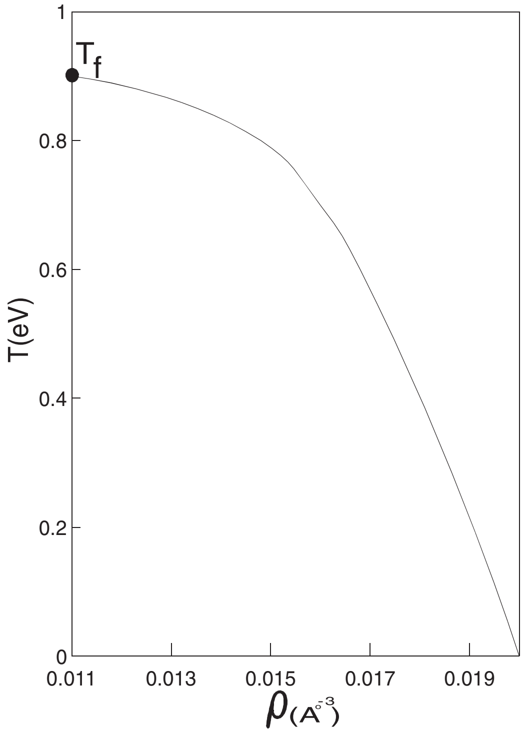

Fig. 6. The densities (A^{-3}) of zero pressure *versus* corresponding temperatures (eV).

parameterize the gas-phase diagram curve by a critical exponent of the form:

$$[\rho_{liquid} - \rho_{gas}]/\rho_c \propto \left| -\frac{1-\mathcal{T}}{\mathcal{T}_c} \right|^{\beta}. \qquad (26)$$

We find that $\beta = 0.384$. This agrees with the corresponding calculation using mean-field theory and Ising model approach ($\beta = \frac{1}{3}$) [20].

Figure 6 shows the densities of zero pressure against their corresponding temperatures. Its is found that the flashing temperature is about 0.6 eV and it occurs at $\rho \approx 0.0166\ \mathrm{A}^{-3}$. This can be, for example compared with Fermi temperature of Na (3.1 eV) and its work function which is approximately about 2.14 eV [21] at $\rho = 0.025\ \mathrm{A}^{-3}$. Here we should mention that $\mathcal{T}_f = 0.6$ eV is the temperature that each electron in uniform electron fluid have to gain to "leave" the positive background, whereas the work function of Na is equivalent to the temperature in which an electron can be removed from the Fermi surface. So one should expect that $\mathcal{T}_w(Na) \gg \mathcal{T}_f$. However, at these temperatures the ions vibrations as well as surface effect should become important which has been ignored in our calculation.

The entropy per electron is presented in Figure 7 as a function of density for different temperatures. As one expected the entropy is falling suddenly respect to density but it is a smooth function of temperature.

From the definition of specific heat per electron *i.e.*

$$C_V = \mathcal{T}\left(\frac{\partial S}{\partial \mathcal{T}}\right)_{\rho} = \left(\frac{\partial E}{\partial \mathcal{T}}\right)_{\rho} \qquad (27)$$

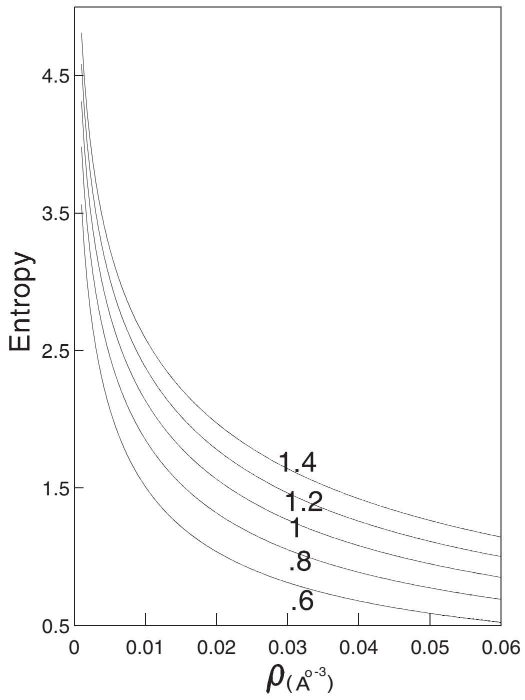

Fig. 7. As Figure 3 but for entropy (eV^{-1}).

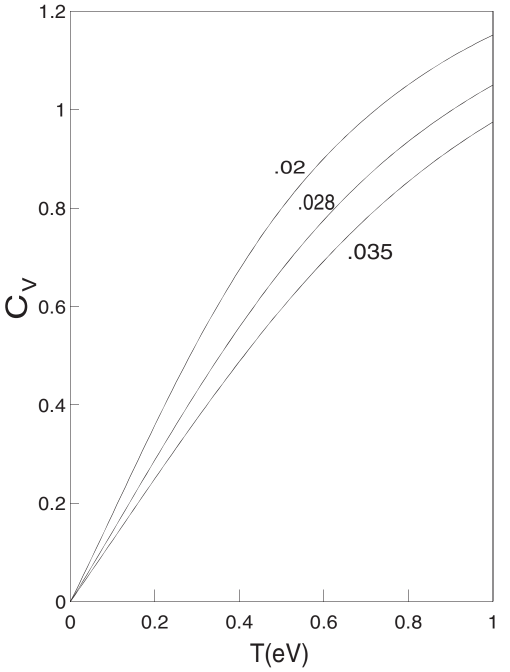

Fig. 8. As Figure 3 but for heat capacity (eV).

we can calculate C_V and plot it against temperature for various densities (Fig. 8). The linear behavior is seen for low temperatures.

Finally two typical correlation functions at zero temperature ($\rho = 0.0156\ \mathrm{A}^{-3}$) and $\rho = 0.01(\mathcal{T} = 0.5)$ and $0.02\ \mathrm{A}^{-3}(1.0$ eV) are given in Figure 9 (10). As it is expected the correlation functions have shorter range as the density (temperature) is increased (decreased). On the

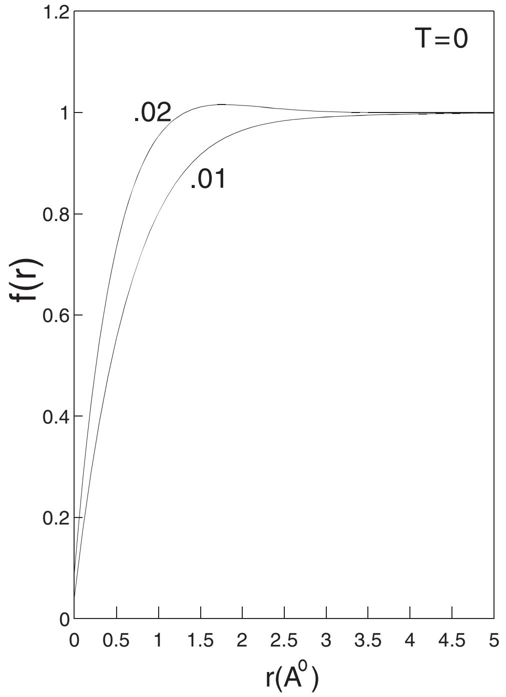

Fig. 9. Two typical correlation functions at $\mathcal{T} = 0.0$ and $\rho = 0.01$ and 0.02 A^{-3}.

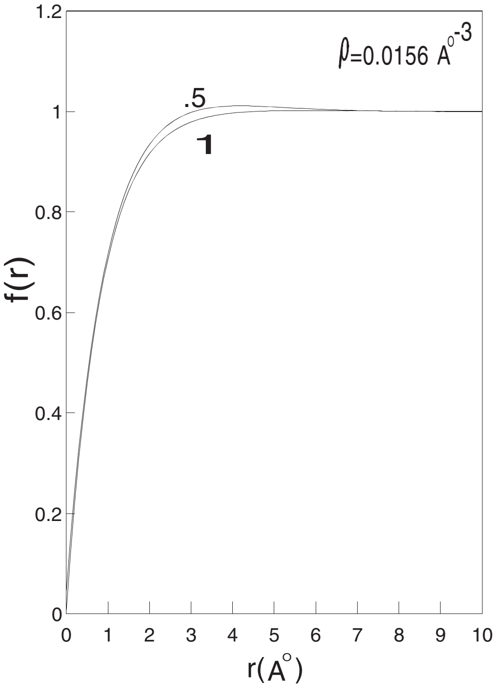

Fig. 10. Two typical correlation functions at $\rho = 0.0156$ A^{-3} and $\mathcal{T} = 0.5$ and 1.0 eV.

other hand at higher densities (temperatures) the correlation functions heal to one with larger (lower) value respect to low (high) densities (temperatures).

In conclusion we have performed a LOCV calculation for uniform electron fluid at finite temperature. It was found that the three-body cluster energy is small. This indicates that the cluster expansion converges rapidly after the two-body term. However, this is not a very serious mathematical criterion for the convergence of cluster expansion series.

It is encouraging that the behavior of our results are very similar to those coming from most sophisticated calculations such as FHNC etc. However, for $r_s > 3$ our ground state energy is 30% higher than the VMC and FHNC calculations. In general for large r_s because of solid phase the choice we have made for the correlation function is not justifies (the same thing is true for other techniques). But in order to get more realistic results we could improve our correlation function in the following ways: (a) The correlation functions have to depend on the momentum of electrons in order to make difference between the correlations deep in the Fermi sea and in the Fermi surface. (b) The three-body correlation can be taken into the account. (c) A full functional minimization of the two-body and three-body cluster energies can be made by solving the Euler-Lagrange differential equations.

The flashing and critical temperatures as well as the heat capacity and critical exponent were found. It was shown that the uniform electron fluid has similar phase diagram to that of nuclear matter and liquid He^3. Finally, it is worth to say that a free energy calculations with LOCV formalism for a given density takes less than few minutes on a Pentium III 450 MHz personal computer.

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