CHAPTER IV

ELECTRICAL CONDUCTIVITY OF METALLIC HYDROGEN

4.1 INTRODUCTION

As we discussed in Chapter I, metallic hydrogen exists initially in a liquid state at pressure 140 GPa and temperature 3000 K. In such a circumstance an electron is not bounded to any proton. We therefore model this system as consists of a degenerated electron gas mixed with classical protons in the ground state. This model corresponds to the framework of Xu and Hansen [9]. Then the Ziman theory [8] of monovalent alkali metals can be applied to this system. Before we calculate the electrical conductivity of this system, the proton-proton radial distribution function and the pseudopotential needed in the Ziman theory must be discussed.

4.2 RADIAL DISTRIBUTION FUNCTION AND FITTING

In the paper by Xu and Hansen [9], the pair correlation in liquid metallic hydrogen was investigated. The ions can be considered as one-component plasma and electrons as jellium model, free electron gas, respectively that constitute a neutral liquid system. The Thomas-Fermi calculation in density functional theory has included the effect of an inhomogeneous electron distribution, the square gradient correction. The radial distribution function is shown in Fig. 4.1. Note that an electron sphere radius $r_S = \dfrac{r}{a_B} = \left(\dfrac{3}{4\pi n}\right)^{1/3}$ where the Bohr radius $a_B = \dfrac{\hbar^2}{me^2}$, $a_1 = r_S Z^{1/3}$, Z is the atomic number and n is the electron concentration.

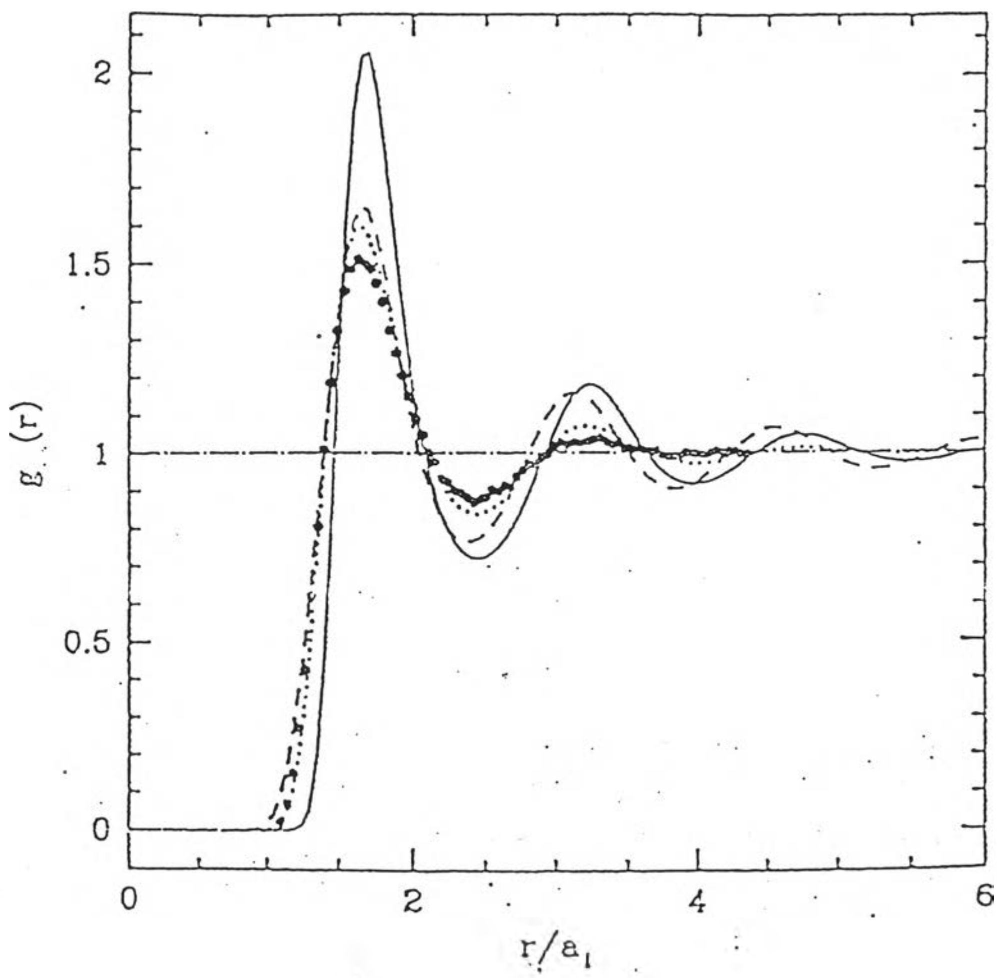


Figure 4.1 The radial distribution function $g(r)$ at 3000 K from the density functional theory. The solid corresponds to $r_s = 0.5$, the dashed line corresponds to $r_s = 1.0$, the dotted line corresponds to $r_s = 1.5$ and the big-dotted line is from molecular dynamics simulation [9].

The other one we use belongs Wier et al. [5], the radial distribution functions to liquid metallic hydrogen for fixed $r_s = 2.0$ at five different temperatures as shown in Fig.4.2.

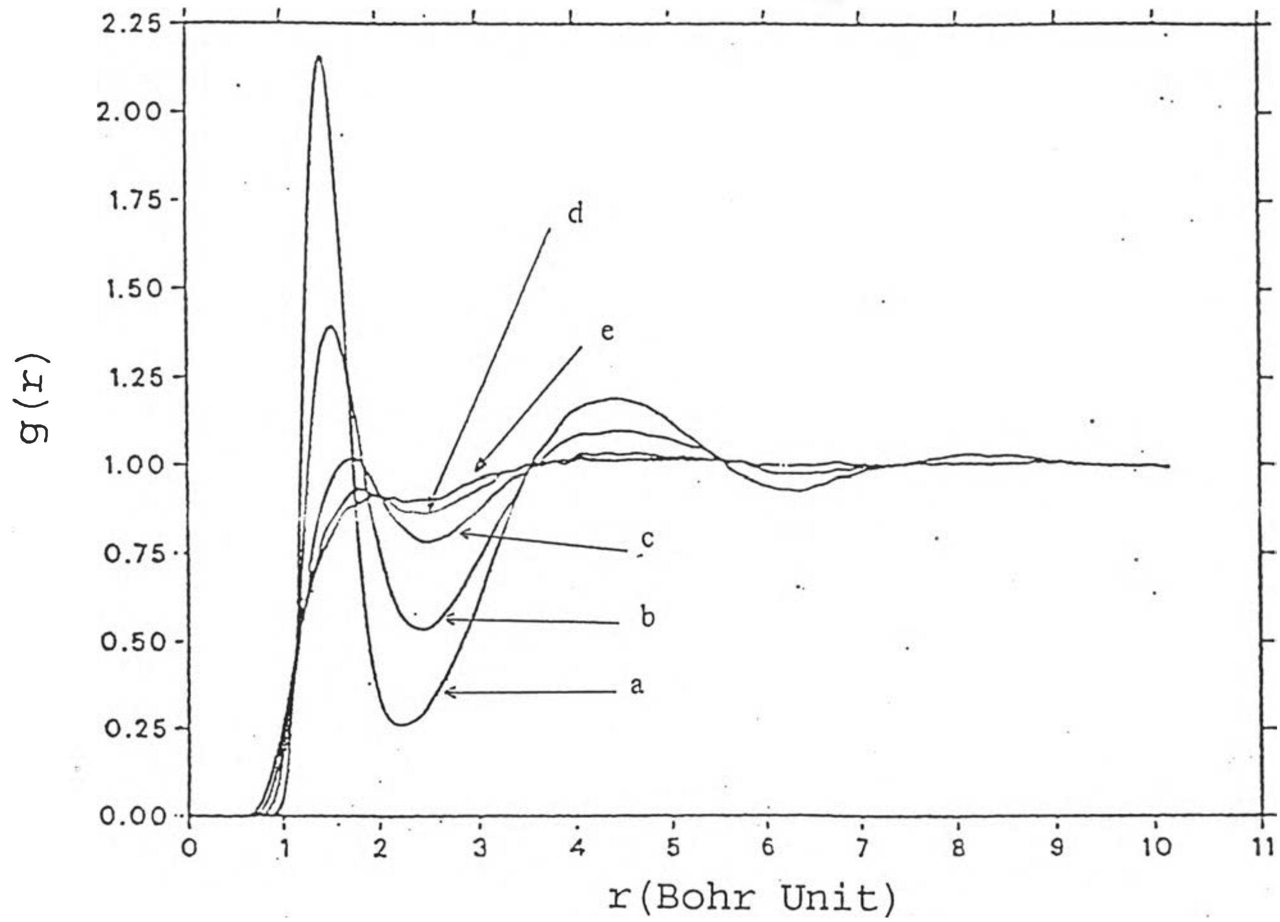


Figure 4.2 Radial distribution functions [5] of liquid metallic hydrogen for fixed $r_s = 2.0$ where a, b, c, d and e corresponds respectively to temperatures 3000, 5000, 10000, 15000 and 20000 K.

To regenerate all numerical values of the radial distribution functions $g(r)$ from Fig. 4.1 and 4.2, we use a fine ruler to measure values of 198 known points of $g(r_i)$ that covers the r_i range $[0,7.5]$. Note that this scale is accurate up to 1/10 of a centimeter then it is suitable to keep only the one decimal point of $g(r_i)$. To complete another point of $g(r)$ from these known points, we apply the 2-point Lagrange interpolation technique [10]

$$g(r)=\sum_{i=1}^{2} g(r_i)\prod_{j\neq i=1}^{2}\frac{(r-r_j)}{(r_i-r_j)}, \qquad (4.2.1)$$

and get numerical points of $g(r)$. These points will be used to calculate the structure factor required in the Ziman theory.

The interpolated result coincides with the non-interpolated one is shown in Fig. 4.3. Note that the another fitting of $g(r)$ curve, least squares fitting, provides us an analytic form of radial distribution function as that described in appendix B.

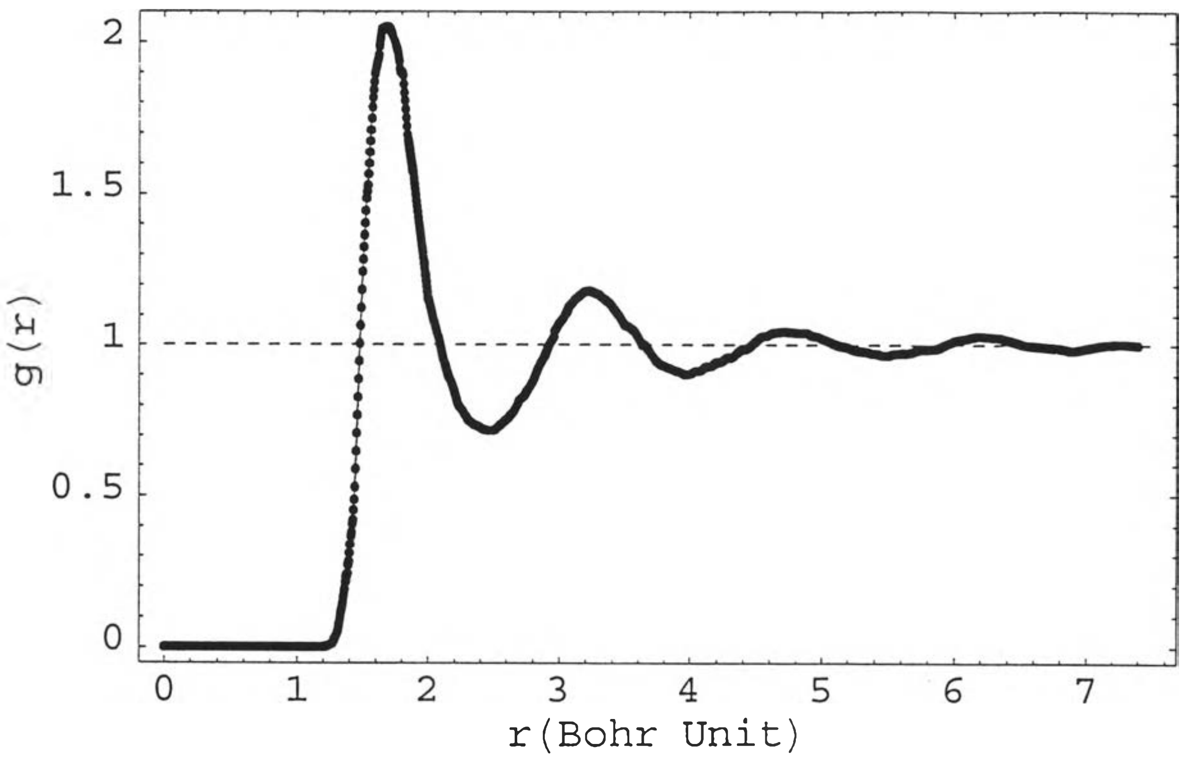


Figure 4.3 The interpolated result of the radial distribution function $g(r)$ fitting by using the 2-point Lagrange interpolation technique, for $r_s = 0.5$ at temperature 3000 K.

4.3 TRIAL PSEUDOPOTENTIAL

In this section we use the concept of pseudopotential to describe the liquid hydrogen system. This potential can be viewed as the second order perturbation direct-indirect Coulomb potential of two metallic atoms [19], the screened Coulomb potential

$$U(R) = \frac{Z^2e^2}{R} exp(-R/\lambda) \tag{4.3.1}$$

where

$\lambda = \frac{\hbar^2 k_F^2}{12nme^2\pi}$,

Z the atomic number,

$k_F = [3\pi^2 n]^{1/3}$ the Fermi wave vector,

R the distance between atoms,

n the electron cocentration,

m electron's mass,

e electron's charge,

$\hbar = \frac{h}{2\pi}$, h Planck's constant,

and its Fourier transform

$$U(K) = 4\pi Z^2 e^2 \left(\frac{\lambda^2}{1+\lambda^2 K^2} \right) \tag{4.3.2}$$

where

K the electron momentum transfers.

The potential (4.3.1) is shown in Fig. 4.4.

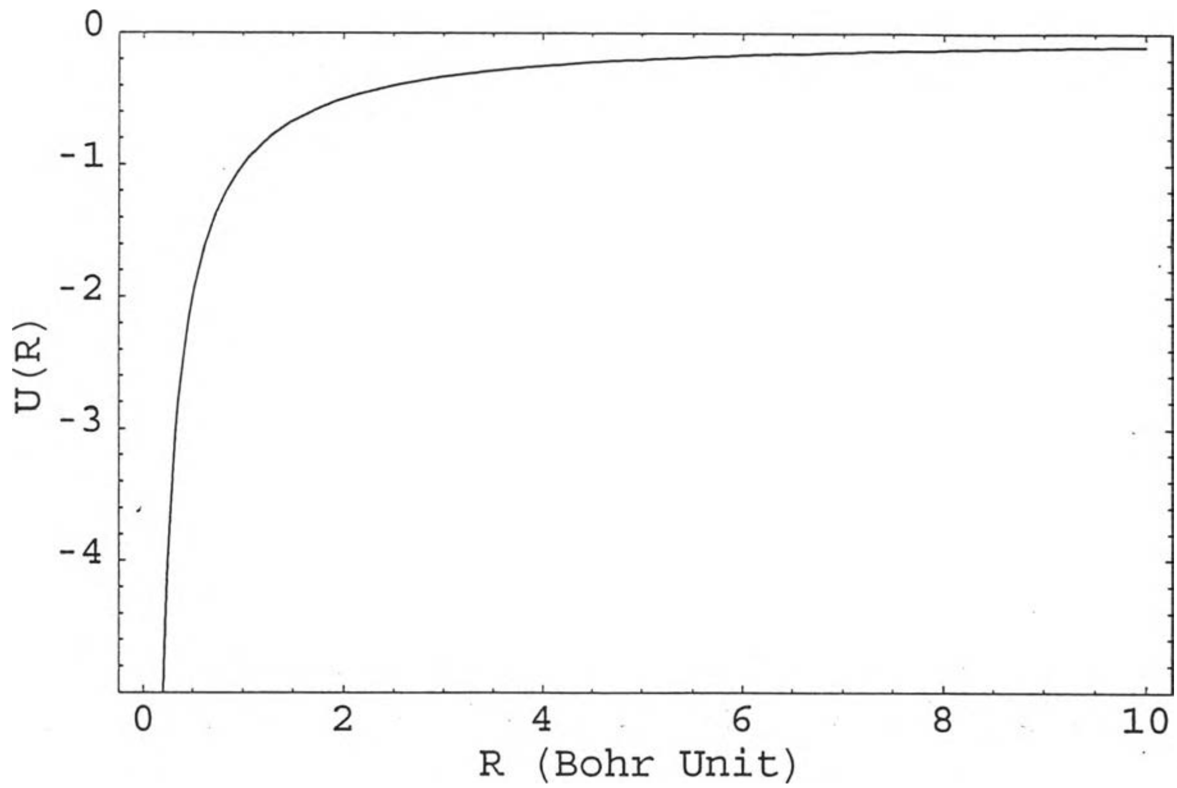


Figure 4.4 A rough drawing of the screened Coulomb potential $U(R)$.

4.4 CALCULATION THE ELECTRICAL CONDUCTIVITY

Before doing any further, we note the meaning of the following variables:

m electron mass,

e electron charge,

n electron concentration,

K electron momentum transfer,

r distance between two atoms,

$g(r)$ the radial distribution function of liquid metallic hydrogen,

$a(K)$ the structure factor of liquid metallic hydrogen,

$U(K)$ Fourier transform of screened Coulomb potential,

$\frac{N}{V}$ proton concentration,

h Planck's constant,

$\hbar = \frac{h}{2\pi}$,

k_F electron wave vector at Fermi surface,

$\upsilon_F = \frac{\hbar k_F}{m}$ electron Fermi velocity,

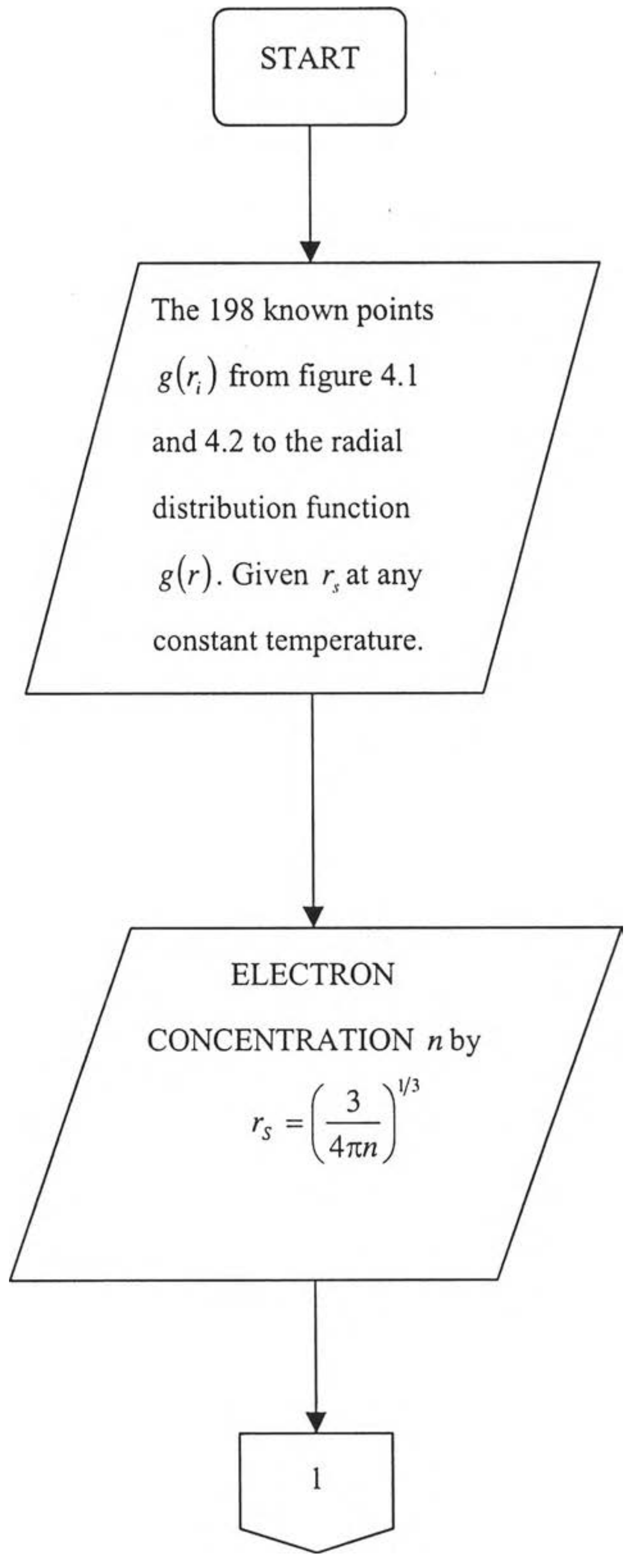
E_F electron Fermi energy,

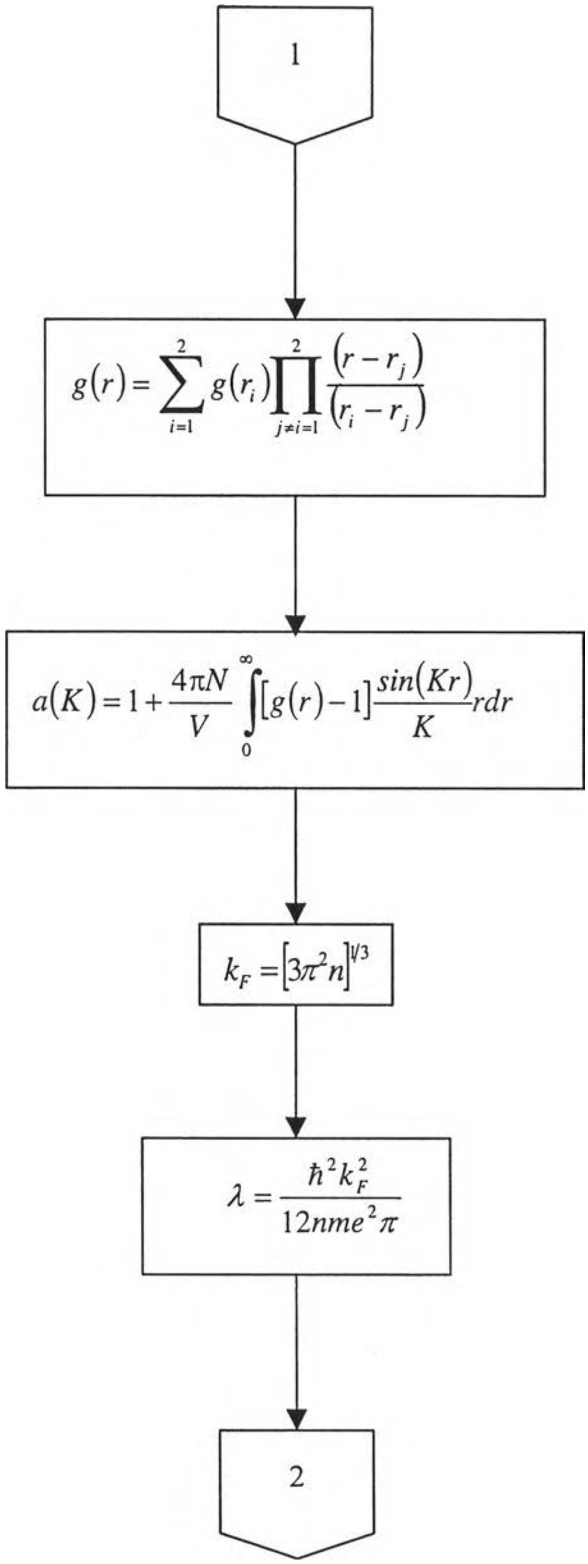
Λ_{lid} electron mean free path and

σ electrical conductivity.

The process of calculating the electrical conductivity of liquid metallic hydrogen is shown by a semi-flowchart as follows:

A semi-flowchart for calculation of electrical conductivity.




1
$g(r)=\sum_{i=1}^{2} g(r_i)\prod_{j\neq i=1}^{2}\frac{(r-r_j)}{(r_i-r_j)}$
$a(K)=1+\frac{4\pi N}{V}\int_0^{\infty}[g(r)-1]\frac{sin(Kr)}{K}rdr$
$k_F=[3\pi^2 n]^{1/3}$
$\lambda=\frac{\hbar^2 k_F^2}{12nme^2\pi}$
2

2

$$U(\mathbf{K}) = 4\pi e^2\left(\frac{\lambda^2}{1+\lambda^2 K^2}\right)$$

$$\langle a\rangle|U|^2 = \frac{1}{4k_F^4}\int_0^{2k_F}|U(\mathbf{K})|^2 a(K)K^3 dK$$

$$E_F = \frac{\hbar^2\left(3\pi^2 n\right)^{2/3}}{2m}$$

$$\Lambda_{liq.} = \frac{\left(2E_F\right)^{3/2}}{3\pi}\frac{1}{\langle a\rangle|U|^2}$$

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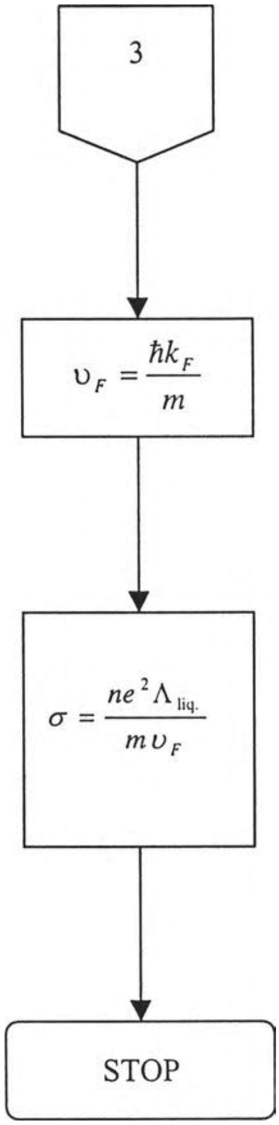
3
$\upsilon_F = \frac{\hbar k_F}{m}$
$\sigma = \frac{ne^2 \Lambda_{\text{liq.}}}{m \upsilon_F}$
STOP

Having given the semi-flowchart, it is easy to convert it into a computer code in the C language. All integrations are accomplished by using the Gauss-Legendre integration technique [10]. Details and computer source codes are provided in Appendix A.

4.5 RESULT

The electrical conductivity of liquid metallic hydrogen is numerically calculated in the previous section. The result of the calculation is shown in Table 4.1 and Fig. 4.5 where the values of the electrical conductivity at various electron concentrations are shown. As for the temperature dependence of σ at fixed $r_s = 2.0$, the result is shown in Table 4.2 and Fig. 4.6.

Table 4.1 The electrical conductivity of liquid metallic hydrogen at various electron concentrations n at T=3000 K. Note that $r_s = (3\pi^2 n)^{1/3}$.

r_s	n $(mol./cm^{-3})$	σ $\times 10^3\ (\Omega\ cm)^{-1}$
0.5	0.52	1.7
1.0	4.19	2.1
1.5	10.41	3.5

Table 4.2 The electrical conductivity of liquid metallic hydrogen at a fixed concentration $r_s = 2.0$ at various temperatures.

T (K)	σ $\times 10^3 (\Omega\, cm)^{-1}$
3000	0.03
5000	0.30
10000	3.03
15000	3.03
20000	3.04

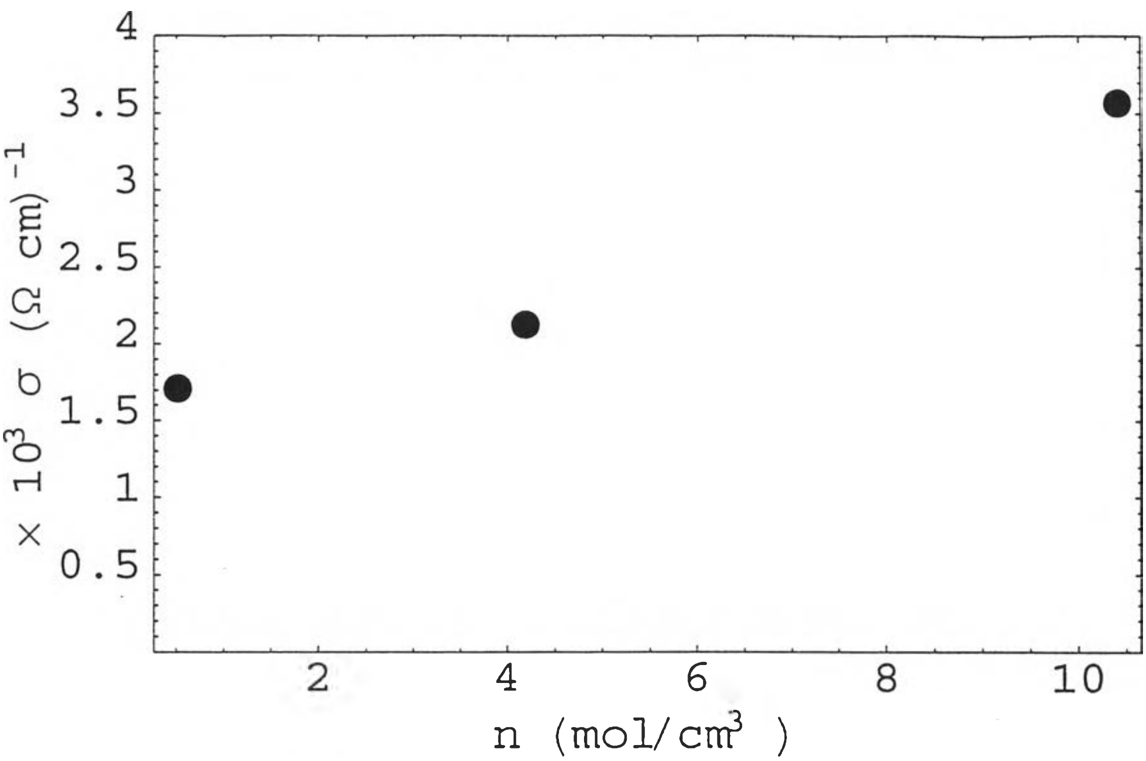

Figure 4.5. The d.c. electrical conductivity of liquid metallic hydrogen for $r_s = 0.5, 1.0$ and 1.5 at temperature 3000 K.

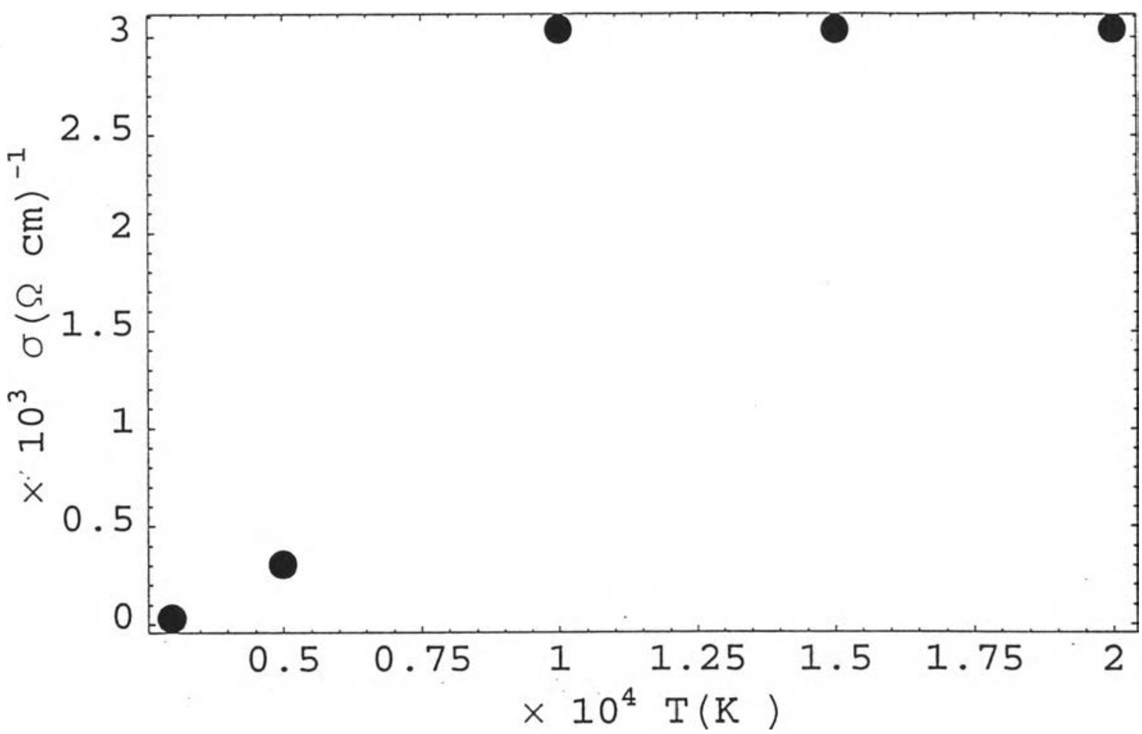

Figure 4.6 The electrical conductivity of liquid metallic hydrogen for $r_s = 2.0$ at various temperatures.

In addition, we compare our electrical conductivity in Fig. 4.5 at the fixed temperature T=3000 K, and with Hensel and Edwards' result [7] at the fixed temperature T= 1750 K as shown in Fig. 4.7. It is clear that the effect of temperatures increases the electrical conductivity.

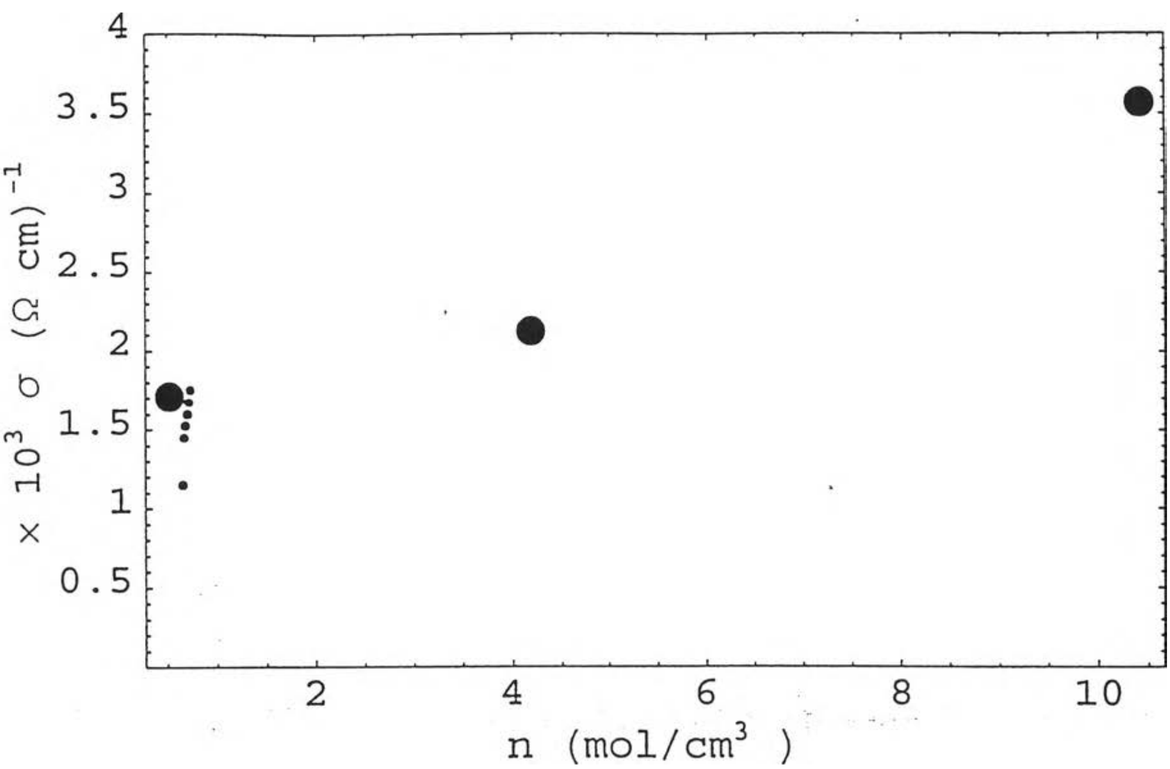

Figure 4.7 The electrical conductivity of liquid metallic hydrogen at two temperatures. Small dots for T=1750 K and big dots for T= 3000 K.