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# A Study of an Integral Equations for Computing Radial Distribution Functions

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# A STUDY OF AN INTEGRAL EQUATIONS FOR COMPUTING RADIAL DISTRIBUTION FUNCTIONS

by

Noraini Ismail

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Submitted to the
Faculty of The Graduate College
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# A STUDY OF AN INTEGRAL EQUATION FOR COMPUTING RADIAL DISTRIBUTION FUNCTIONS

Noraini Ismail, M.A.

Western Michigan University, 1988

A two parameter integral equation, equation T is studied to compute radial distribution functions for a classical fluid whose single component particles interact pairwise acording to a square-well potential function. A computer program originally written for a DEC 10 was modified to run on a DEC VAX. At the same time, modifications were made to take advantage of the faster VAX and to reduce the time an operator must spend to get a solution to the integral equation. Solutions were obtain for several densities, temperatures, and parameter values. Temperatures ranged from a high temperature gas to near critical temperatures. Accurate results were easily obtained for medium and high temperatures but derivations from 'exact' results occured at low temperatures and high densities.

# ACKNOWLEDGEMENTS

First of all, I would like to thank God for without His strength and will this study could have never been completed. I would also like to take this opportunity to express my deepest gratitude to late Dr. David Carley for his patience and guidance throughout the entire study and my regret that he didn't have the opportunity to see the finished version of this written work. To both of my parents, I would like to express my appreciation for everything that they have done for me and for making me what I am today. I would like to thank all of my special "sahabah" for being so supportive and for keeping up with me during my difficult periods. Finally, I would like to thank the entire faculty and staff of the Department of Physics for giving me great opportunity to gain knowledge here at Western Michigan University and for making my stay here in Kalamazoo such a memorable experience.

Noraini Ismail

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# CHAPTER I

# INTRODUCTION

Statistical Mechanics deals with the understanding of microscopic behavior of individual molecules that makes up a system and the connection that can be established from this knowledge with macroscopic behavior. It is a goal to obtain equations of state for all substances. Practically this goal is not possible since representation and description of interparticle forces are not complete.

For some systems, the molecular interactions are neglected due to their simple or no structure conditions that make their molecules evenly distributed. Such systems are of low density gases. They follow the ideal gas equation of state,

$$PV=NkT \tag{1}$$

where P is the pressure, V is the volume, N is the number of molecules, k is the Boltzman's constsnt and T is the absolute temperature. But for other system, such as in cases of dense gases and liquids, the molecular interactions become more important and more complicated and it is necessary to use approximations before any significant progress can be made to find equations of state. The Van Der Waals equation is an improvement over the ideal gas equation where it takes into account the intermolecular interactions,

$$\left(P + \frac{a}{\tilde{v}^2}\right)(\tilde{v} - b) = RT \qquad (2)$$

where,

$R$ = gas constant = $N_a k$,

$$\tilde{v} = \frac{N_a v}{N},$$

$N_a$ = Avogadro's number,

and a and b are parameters depending upon the type of molecule. However, the Van Der Waals equation does not accurately represent any real substance.

In this study radial distribution functions are solved from integral equation T and are used to find equations of state for pressure P and internal energy U. The radial distribution function is related to the probability of finding a molecule at a distance r from a central molecule. For the case of an ideal gas $g(r) = 1$, the distribution is uniform. For real fluids, $g(r) = 0$ distance is less than the molecular diameter.

The force between molecules with separation r, can be written as

$$F(r) = -\frac{d\bar{\Phi}}{dr} \qquad (3)$$

The general form of potential energy and the form of force are shown below,[1]

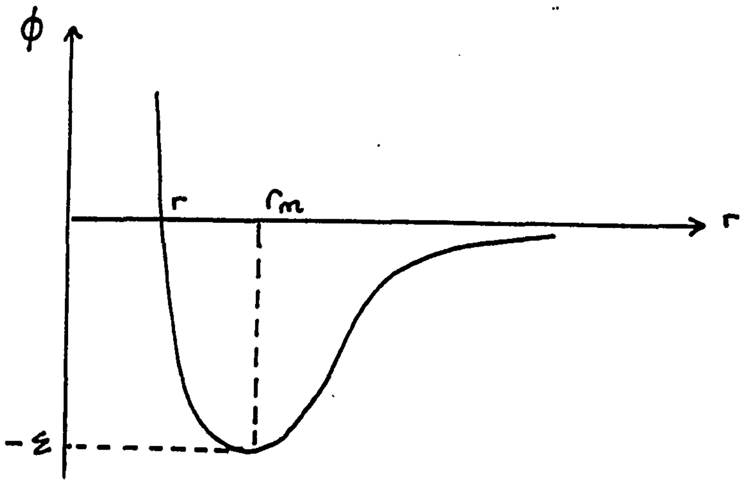

Figure 1. General Form of Potential Energy.

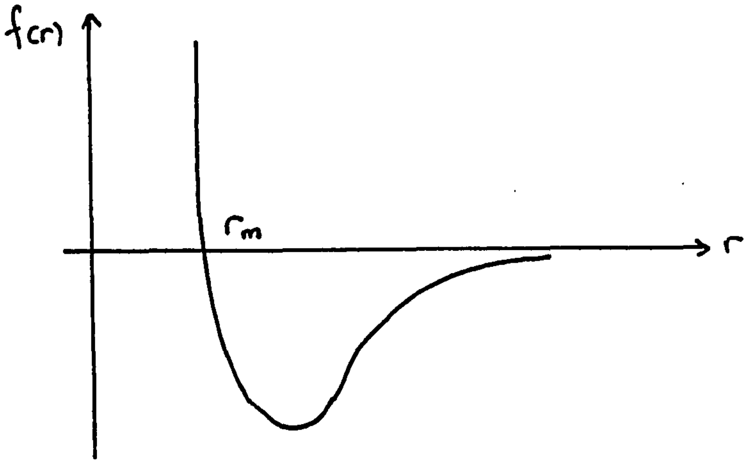

Figure 2. General Form of Force.

In this study, the simplified potential square-well function is used in the evaluation of the integral equation T. It is more realistic than the hard sphere since it considers both the attraction and the repulsive forces in the interaction of the molecules. It is the objective of this study to find the best choice parameters of integral equation T. This equation is then used to obtain radial distribution functions to get pressure and internal energy equations of state.

# CHAPTER II

## THE SYSTEM

When selecting a system, we come to a choice of a real fluid or a hypothetical fluid. The hypothetical fluid is an assumed well defined model of fluids that describes how process between particles should act. In our study, we consider only simple classical fluids. It is a system of spherically symmetric particles with only radial forces acting between them. "Classical" means that it can be adequately described by classical mechanics and no quantum mechanics are needed. The potential energy of this system can be represented as sum of pair interaction,

$$N = \sum_{i>j} \phi ( r_{ij}) = \sum_{i>j} \phi_{ij} \tag{4}$$

where $r_{ij}$ is the separation distance between particle i and j and is the pair potential energy. But when we consider real systems, the interaction becomes more than pair interactions, so that the energy expression above becomes,

$$N = \sum_{i>j} \phi_{ij} + \sum\sum_{i>j>k} \phi_{ij} + \dots \tag{5}$$

where the higher order terms become significant at higher densities.

The nature of this study concerns the condition for which the computational techniques work and because of this we choose the hypothetical fluids. In a study of real fluids there are discrepencies between theory and experiment which arise from inadequate theory and from a poor description of the particle interactions, it is usually difficult to identify the source of error.

In our case, the square-well potential was chosen because it has some of the characteristics of the real molecular potential and it has been extensively studied by other theoretical methods, so that we have basis for comparison. Also some success has been achieved in computing thermodynamic equations of state when real fluids are represented by simple classical fluids.

In a simple classical fluid the Hamiltonian is of the form,

$$H = K + \Phi = K + 1/2 \sum_{i} \sum_{j} \phi ( r_{ij} ) \tag{6}$$

where K is the kinetic energy of the particles expressed in terms of their momenta,

$\Phi$ is the potential energy of the particles,

$\phi$ is the pair potential energy which is assumed to be a function of their separation distance only.

We assume a system of particles having a potential energy equal to the sum of pair potential energies of the form,[2]

$$
\begin{aligned}
&\phi(r) = \infty && r < d \\
&\phi(r) = -\varepsilon && d \le r \le Kd \\
&\phi(r) = 0 && r > Kd \qquad (7)
\end{aligned}
$$

where d is the diameter of the molecule, K is the parameter for the width of the well (which is to be taken in this case to be 1.5), is the depth of the well, r is the separation distance of a pair of particles, and ø is the pair potential energy. The shape of this potential function is shown in Figure 3 below.

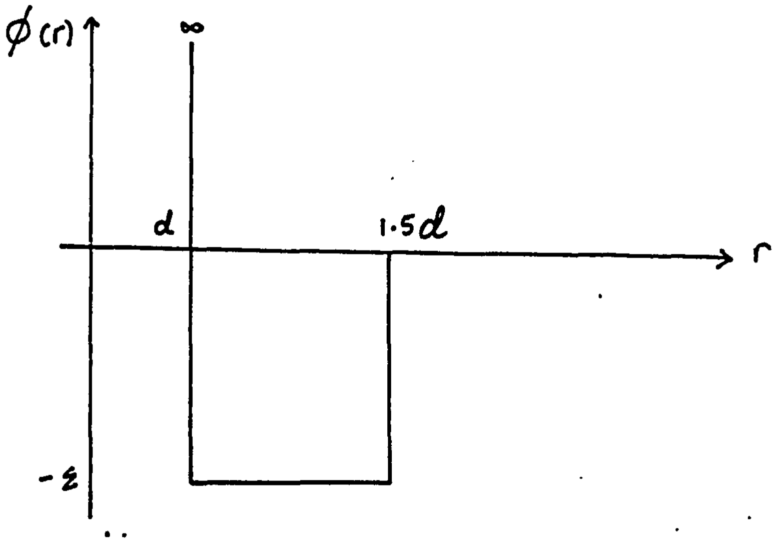

Figure 3. Square-Well Potential Function.

Below are the dimensionless quantities being used,[3]

$$x = \frac{r}{d} \qquad (8)$$

$$T^* = \frac{kT}{\varepsilon} = \frac{1}{\beta\varepsilon} = \frac{1}{\theta^*} \qquad (9)$$

$$n^* = \frac{Nd^3}{V} \tag{10}$$

where k is Boltzmann's constant, T is the absolute temperature and N is the number of particles in volume V.

The square-well potential is useful in this study as a test of the effectiveness of our proposed parametric integral equation since many theories have been applied to this model.

## Radial Distribution Function and the Thermodynamic Equations

The average number density n(r) about a given particle is, in general, not constant in a classical one component fluid having an average number density,

$$\bar{n} = \frac{N}{V} \tag{11}$$

where N is the number of particles and V is the volume. The radial distribution function g(r) is defined as the factor by which n(r) differs from n according to,

$$n(r) = \bar{n}\, g(r), \tag{12}$$

From the Maxwell-Boltzmann distribution law g(r) for a simple classical fluid can be written as,

$$g(r) = V^2 Z^{-1} \int_V \ldots \int \exp(-U/kT)\, d\underset{\sim}{r}_3 \ldots d\underset{\sim}{r}_N,$$

where $$Z = \int_V \ldots \int \exp(-U/kT)\, d\underset{\sim}{r}_1 \ldots d\underset{\sim}{r}_N \, , \qquad (13)$$

in the limit as N approaches infinity, where U is the potential energy and the integration is over the position coordinates of the particles. Figure 4 shows the typical shape of a radial distribution function. It gives an indication of the stucture of the molecule distribution as related to the origin. The structure in a dense gas or liquid is correlated to the origin molecule only over a short distance. Beyond that point it is unaffected.

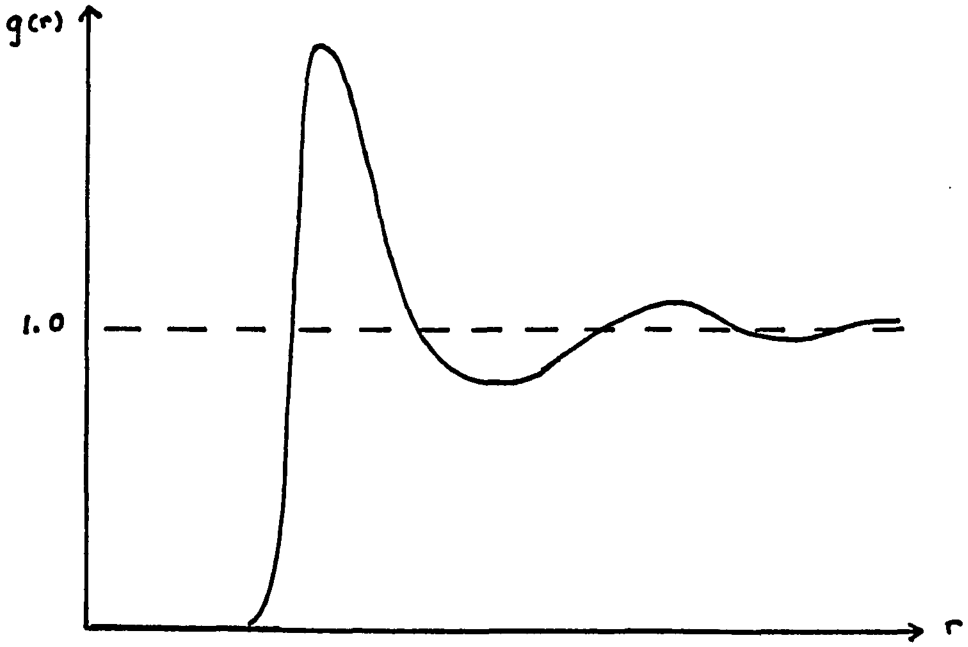

Figure 4. Radial Distribution Function

The radial distribution as a power series in densities can be written as,

$$g\, e^{(ß\o)} = 1 + \sum_{k=3}^{\infty} \frac{\bar{n}^{(k-2)}}{(k-2)!} \int \ldots \int \Big( \sum_{(QK)} \prod f_{ij} \Big)\, d\bar{r}_3 \ldots d\bar{r}_k \qquad (14)$$

where $f_{ij}$ is the Mayer function defined as,

$$f(r_{ij}) = e^{(-ß\o(r_{ij}))} - 1 \tag{15}$$

where $r_{ij}$ is the distance between molecule i and j. Thermodynamic quantities can be calculated from integration once g(r) and ø(r) are known. The general equation for pressure is[4]

$$P^* = \frac{PV}{NkT} = 1 - \frac{2\pi N}{3VkT} \int_0^\infty \left(\frac{d\o}{dr}\right) g(r)\, r^3\, dr, \tag{16}$$

For the square-well studied here, the well is taken between x = 1 and x = 1.5. This reduces the above expression to,

$$P^* = 1 + \frac{2}{3}\pi n^* \,[\, g(1) - 3.375\, g(1.5)\, (1 - e^{-\theta^*})\,] \tag{17}$$

where g(1) is the radial distribution function as x approaches 1 from above and g(1.5) is the value as x approaches 1.5 from below.

The general equation for internal energy is,[5]

$$U^* = \frac{2v}{3NkT} = 1 + \frac{4\pi N}{3VkT} \int_0^\infty \o(r)\, g(r)\, r^3\, dr \tag{18}$$

and it reduces to,

$$U^* = 1 - \frac{4\pi n^*}{3T^*} \int_1^{1.5} g(x)\, x^2\, dx \tag{19}$$

The derivation of both simplified thermodynamic equations, P* and U*, can be found in Appendix D.

## Methods of Obtaining g

Two basic methods are used to calculate g(r), other than integral equation, i.e, the so-called "exact" method and the pertubation method.

### Molecular Dynamic Method[6]

In this method, Newton's equations of motion are solved as the system evolves in time. The system consists of cells with a known amount of molecules (approximately 1000). Initial configuration such as position, potential and kinetic energies are specified for each molecule in a cell and the surrounding cells. These surrounding cells are considered to be image particles for each of the N particles in the basic cells. The number of particles in each cell is kept constant so that as a molecule leaves a cell, another molecule from a neighboring cell will enter. To avoid correlation between molecule entering and exiting the cell, truncation have to be done. Several collisions per molecule are required before the transient effects of the starting configuration have died out. As the time goes, the movement of the molecules gives new positions and new velocities. From theis information the pressures, internal energies and other thermodynamic properties are determined. This method uses the microcanonical ensemble where total energy is held constant and temperature is allowed to fluctuate.

## Monte Carlo Method[7]

In this method the same cells with a fixed number of molecules are again used. Instead of solving Newton's equation of motion, a probability rule is used for particle movement. One of the N particles is chosen at random and given a new random position chosen uniformly within the cell. If movement causes a decrease in configurational energy, the movement is accepted or allowed. But if there is an increase in energy, the movement is also allowed with probability of

$$P = \exp \frac{(-\Delta U)}{kT} \qquad (20)$$

where $\Delta U$ is the change in potential energy between two configurations. The probability is then compared to a random number selected from 0 to 1. If the probability is greater than this random number, the particle is moved and if it is less, the movement is rejected. Whether the movement is successful or not, the contribution of the resulting configuration to the average being computed is included. The above process is repeated many times and finally the thermodynamic properties of the system are determined. Notice that unlike the case of the molecular dynamics method, the movement of molecules in the Monte Carlo method does not represent physical motions. The movement of molecules is done only to provide a sampling over which averages can be made. Monte Carlo uses the canonical ensemble which holds temperature constant and allows the energy to fluctuate.

The Monte Carlo together with Molecular Dynamic methods are often considered to be exact because they are the most direct means of computing g(r) and they also provide dependable results at several densities (intermediate and high densities) for which integral equations often yield large errors. The results are often used to test other less direct methods such as integral equations and pertubation methods. Major disadvantages are that this method needs large computing times and limits the number of degrees of freedom considered. One thing should be kept in mind; there are approximations involved in these methods and it is still prudent to study thermodynamic systems from several points of view.

## Pertubation Method

This method is basically the modern Van Der Waals theory, and it is proven to be a successful theory when properties of systems such as hard-sphere are known accurately enough. The basic idea behind this method is to separate the attractive and repulsive interactions. However Maitland (cited in Oxford, 1981) stated:

> It is postulate that the structure of simple dense fluids is chiefly determined by the repulsive intermolecular interactions and that the attractive forces maintained the high density, but do not otherwise have much effect on the structure, as described by radial distribution function, g(r). Both hard-sphere and Lennard-Jones liquids has similar radial distribution functions, which suggest that the effect of the repulsive interactions may be modeled with reasonable accuracy using hard-sphere system of suitable diameter. (p. 32)

The pair potential energy is the sum of the reference potential and the pertubation potential,

$$u(r) = u_0(r) + u_1(r) \tag{21}$$

The configurational partition function for pertubation theory is,[8]

$$Z_Q = \frac{1}{N!} \int \ldots \int \exp \left[ \frac{-1}{kT} \sum_{i>j} u_0(r_{ij}) + u_1(r_{ij}) \right] dr_1 \ldots dr_N \tag{22}$$

With few substitutions, the equation of state, which consists of reference system and pertubation contributions, can be obtained.

$$P = \underbrace{P}_{\text{reference system}} + \underbrace{\frac{2\pi N}{3} \frac{\partial}{\partial v} \left[ \frac{1}{v} \int u(r)\, g(r)\, r\, dr \ldots \right] + \text{higher terms}}_{\text{pertubation contributions}} \tag{23}$$

The division of u(r) into reference and pertubation potentials determines the success of the results.

Other pertubation methods used hard-sphere (with diameter d) for the reference potential and Lennard-Jones (with a slightly greater diameter) for the pertubation potential. By making the hard-sphere diameter a function of temperature, it is found that the diameter decreases with increasing temperature. Pertubation method can also combined with integral equation methods, and it provides a valuable source of information on properties of fluids.

## Integral Equations

Approximate integral equations to calculate the radial distribution function offer an alternative way to determine thermodynamic functions. They work well and give good results at low densities but large errors sometimes occur at intermediate and high densities.

The total correlation function is a measure of the variation about the uniform densities caused by the reference molecule at the origin. It relates to the radial distribution function as,

$$h(r) = g(r) - 1 \tag{24}$$

and to the direct and indirect correlation function by means of the Ornstein-Zernike equation,[9]

$$\underset{\text{total}}{h(r_{12})} = \underset{\text{direct}}{c(r_{12})} + n \underset{\text{indirect}}{\int c(r_{13})\, h(r_{23})\, dr_3,} \tag{25}$$

Figure 5 shows the typical correlation function.

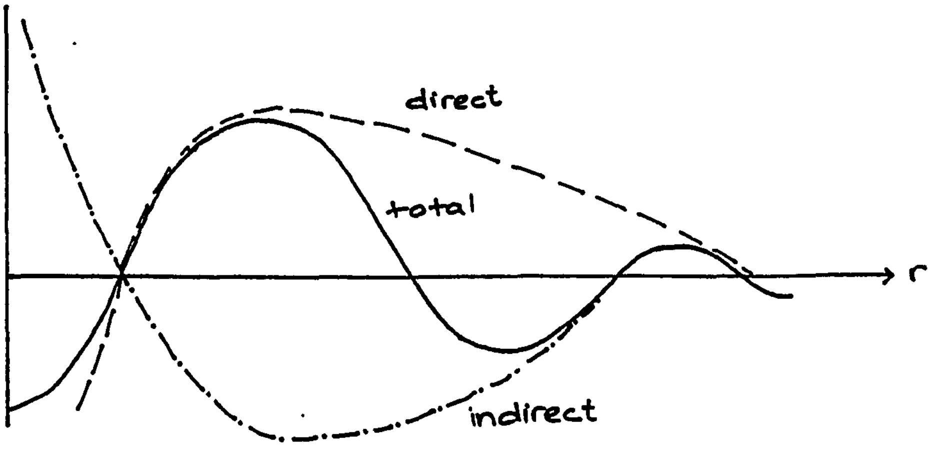

Figure 5. Correlation Function.

The direct correlation can be written in terms of a density expansion as,[10]

$$c(ij) = \sum_{a\geq 1} \alpha_{a+1}\ (ij)\ n^{-a-1} \tag{26}$$

where,

$$\alpha_{a+1}\ (ij) = \frac{1}{(a-1)!} \int \dots \int \Sigma \Pi f(ij)\ dr_3 \dots dr_{N-1}$$

We define S to be

$$S = h(r) - c(r) = g(r) - 1 - c(r) \tag{27}$$

Approximate integral equations are obtained by assuming a relationship between c and g or between S and g. Some of the integral equations which have been intensively studied are listed below.

(Percus Yevick) $c = g\,(1 - e^{\beta\phi})$ (28)

(Hypernetted) $c = g - 1 - \ln(ge^{\beta\phi})$ (29)

(Equation C) $c = g - 1 - (1/a) \ln (age^{\beta\phi} - a + 1)$ (30)

(Equation T) $c = e^{-\beta\phi} (1 + S + b_2 S^2 + b_3 S^3) - 1 - S$ (31)

Using c, the correlation function, and substituting it onto the compressibility equation of Ornstein and Zernike, an equation of state can be determined,[11]

$$\frac{1}{kT}\left(\frac{\partial P}{\partial \bar{n}}\right) = 1 - 4\pi \bar{n} \int_0^\infty c(r)\, r^2\ dr \tag{32}$$

In terms of S and the density expansions we for have the radial distribution function,

Percus-Yevick equation

$$g = e^{(-\beta \phi)} (1 + S) \tag{33}$$

Equation C

$$g = e^{(-\beta \phi)} ( 1 + 1/a ( e^{aS} - 1) )$$
$$g = e^{(-\beta \phi)} ( 1 + S + 1/2\, aS^2 + 1/6\, a^2 S^3 + \dots ) \tag{34}$$

Hypernatted Chain Equation

$$g = e^{(-\beta \phi)}\, e^{S} \tag{35}$$
$$= e^{(-\beta \phi)} ( 1 + S + 1/2\, S^2 + 1/6\, S^3 + \dots )$$

Equation T

$$g = e^{(-\beta \phi)} ( 1 + S + b_2 S^2 + b_3 S^3 ) \tag{36}$$

Equation N

$$g = e^{(-\beta \phi)} ( 1 + S - ( a - 1 ) S^2 + ( a - 1 )^2 S^3 + \dots ) \tag{37}$$

where a, $b_2$, and $b_3$ are adjusted parameters. The general form of these equations is,

$$g = \exp(-\beta \phi)(1 + S + b_2 S^2 + b_3 S^3 + \ldots) \qquad (38)$$

There are similarities among these equations when we examine them. Equation C is the same as PY equation when $a = 0$ and is the same as the HNC equation when $a = 1$. Equation T is the same as PY equation when $b_2 = b_3 = 0$ and is similar to ( but not exactly the same as ) the HNC equation when $b_2 = 1/2$ and $b_3 = 1/6$.

# CHAPTER III

## COMPUTATIONAL METHOD

The computer program used to solved equation T numerically is run on a digital computer. The method of solution used for this purpose is essentially that of Broyles.[12] It is an iterative procedure using the Fourier transform of the function S,

$$\tilde{S}(k) = \frac{1}{2\pi} \iiint S(\vec{r}) \exp(i\vec{k}.\vec{r})\, d\vec{r} \tag{39}$$

Part of this research involved modifying an old computer program written for the DEC 10 so that it would run on the DEC VAX. This program solves the integral equations to obtain radial distribution functions, using an iteration technique. At the same time the program was modified to improve an extrapolation technique and to reduce the time it takes an operator to obtain a solution. To make sure that the changes didn't effect the whole program, sample values were tested from previously known results. More detailed explanations of these improvements are in Appendix B.

Good convergence is easy to get at low density with a small number of iterations. At high density, longer time is needed and solutions become more sensitive to the interval width in the representation of the function.

All of the solutions obtained for g(r) were done through the iteration process. From g(r) the pressure $P^*$ and internal energy $U^*$ are calculated for several densities using the equations for the square-well potential,

$$P^* = 1 + \frac{2}{3}\pi n^* \left[ g(r) - 3.375\, g(r) \left( 1 - e^{-0^*} \right) \right] \qquad (17)$$

$$U^* = 1 - \frac{4 \pi n^*}{3T^*} \int_{1.0}^{1.5} g(x)\, x^2\, dx \qquad (19)$$

We note that the pressure is more sensitive to the change of parameters than internal energy. For a given $n^*$ and $T^*$, the dependence of $P^*$ and $U^*$ upon equation T parameters are approximated,

$$P^* = P_0^* + C_1 b_2 + C_2 b_3 + C_3 b_2^2 + C_4 b_3^2 + C_5 b_2 b_3 \qquad (40)$$

$$U^* = U_0^* + C_1 b_2 + C_2 b_3 + C_3 b_2^2 + C_4 b_3^2 + C_5\, b_2\, b_3 \qquad (41)$$

where $P_0^*$ and $U_0^*$ are the pressure and internal energy values obtained whe $b_2 = b_3 = 0$. By solving the integral equation for at least six sets of parameters, the values of C's may be obtained using the method of least squares. Once the C's are obtained, it is possible to determine the values of $b_2$ and $b_3$ which will give a specified $P^*$. By plotting a graph of $b_2$ versus $b_3$ which gives correct values of $P^*$ for a fixed $T^*$ and different values of $n^*$, one can hope to obtain the best values of $b_2$ and $b_3$ for the given isotherm. The radial distribution function is again solved using these best values of $b_2$ and $b_3$ for a few densities and these results are used in the interpolation formula,[13]

$$P^* = \frac{(1 + a_1 n^* + a_2 n^{*2} + a_3 n^{*3})}{(1 + a_4 n^* + a_5 n^{*2} + a_6 n^{*3})} \tag{42}$$

$$U^* = \frac{(1 + a_1 n^* + a_2 n^{*2} + a_3 n^{*3})}{(1 + a_4 n^* + a_5 n^{*2} + a_6 n^{*3})} \tag{43}$$

Graphs are plotted and comparisons are made to the "exact" values and values of equation C. All computer programs for the computation are listed in Appendix B.

# CHAPTER IV

## RESULTS AND COMPARISONS

The major task involved is to find solutions to the integral equation T at seven suggested temperatures T* that ranged from near critical temperature to high temperatures in the gas region using the computer program. Radial distribution functions g(x) are solved for two groups of discrete points with fixed intervals. 75 points are used to specify the function with an interval of $\Delta x = 0.07142857$, while 297 points are used to specify the function with an interval of $\Delta x = 0.01785714$. At each temperature the pressure P* and the internal energy U* are determined from radial the distribution functions calculated.

### Results for Temperature $T^* = 3.3333$

First, solutions for several sets of parameters with fixed n* were obtained. Results for this isotherm at $n^*=0.85$ and $n^*=0.65$ are shown in Table 1, where only 297 points solutions are shown. More complete results can be found in Appendix A.

Table 1

P* and U* Using Equation T at T* = 3.3333

| $b_2$ | $b_3$ | n* | P* | U* |
|---|---|---|---|---|
| 0 | 0 | 0.85 | 7.15 | -0.191 |
| 0 | 0.1667 | | 8.50 | -0.185 |
| 0.5 | 0 | | 8.81 | -0.189 |
| 0.1775 | 0.0092 | | 7.45 | -0.189 |
| 0.4 | 0.05 | | 8.80 | -0.187 |
| 0.5 | 0.1667 | | 9.46 | -0.185 |
| 0.3 | 0.3 | | 9.54 | -0.181 |
| | | | | |
| 0 | 0 | 0.65 | 3.58 | 0.070 |
| 0 | 0.1667 | | 3.79 | 0.072 |
| 0.5 | 0 | | 4.05 | 0.076 |
| 0.1175 | 0.0092 | | 3.72 | 0.072 |
| 0.4 | 0.1667 | | 4.18 | 0.077 |
| 0.3 | 0.3 | | 4.15 | 0.076 |

We established first "exact" results which come from the Monte Carlo studies of Rottenberg[14] at T* =3.3333 for medium and high density and Carley's[15] results of parametric integral equation C for low density as shown in Table 2. The results were then used to find the constants in the interpolation formulas, equation (42) and equation (43). The interpolated "exact" results and their corresponding Pade' coefficients are shown in Table 3.

Table 2

"Exact" Results Used for $T^* = 3.3333$

| Source | $n^*$ | $P^*$ | $U^*$ |
|---|---|---|---|
| Carley's results of parametric integral equation C | 0.001 | 1.0003559 | 0.9986568 |
| | 0.05 | 1.00223 | 0.93304 |
| | 0.10 | 1.0553 | 0.86620 |
| | 0.15 | 1.1016 | 0.79905 |
| | 0.20 | 1.65 | 0.7312 |
| | 0.25 | 1.249 | 0.6625 |
| | 0.30 | 1.360 | 0.5923 |
| | 0.35 | 1.506 | 0.5207 |
| Monte Carlo results of Rottenberg | 0.424 | 1.72 | |
| | 0.591 | 2.76 | |
| | 0.750 | 5.10 | |
| | 0.820 | 6.72 | |
| | 0.853 | 7.84 | |
| | 0.890 | 9.06 | |
| | 0.918 | 9.60 | |
| Results as read from Alder's graph. | 0.2828 | 1.32 | 0.61 |
| | 0.3536 | - | 0.52 |
| | 0.4714 | - | 0.35 |

Table 2--Continued

| Source | n* | P* | U* |
|---|---|---|---|
| Results as read from Alder's graph. | 0.5657 | 2.58 | 0.20 |
| | 0.7071 | 4.42 | 0 |
| | 0.7857 | 5.78 | -0.18 |
| | 0.8319 | 6.98 | -0.20 |
| | 0.8839 | 8.80 | -0.28 |

Table 3

Interpolated "Exact" Results for T* = 3.3333 With Corresponding Padé Coefficients

| n* | P* | U* |
|---|---|---|
| 0.05 | 1.022 | 0.933 |
| 0.10 | 1.055 | 0.866 |
| 0.15 | 1.102 | 0.799 |
| 0.20 | 1.164 | 0.731 |
| 0.25 | 1.249 | 0.662 |
| 0.30 | 1.366 | 0.593 |
| 0.35 | 1.895 | 0.523 |
| 0.40 | 1.611 | 0.452 |
| 0.45 | 1.845 | 0.308 |
| 0.50 | 2.127 | 0.235 |
| 0.55 | 2.480 | 0.161 |

Table 3--Continued

| $n^*$ | $P^*$ | $U^*$ |
|---|---|---|
| 0.60 | 2.925 | 0.086 |
| 0.65 | 3.488 | 0.011 |
| 0.70 | 4.20 | -0.06 |
| 0.75 | 5.10 | -0.354 |
| 0.80 | 6.237 | -0.227 |
| 0.85 | 7.666 | -0.306 |
| 0.90 | 9.447 | -0.386 |

Pade' Coefficients

| $P^*$ | $U^*$ |
|---|---|
| $a_1 = -3.959$ | $a_1 = 4.436$ |
| $a_2 = 4.989$ | $a_2 = -17.17$ |
| $a_3 = -5.014$ | $a_3 = 12.82$ |
| $a_4 = -4.313$ | $a_4 = 5.78$ |
| $a_5 = 4.798$ | $a_5 = -9.606$ |
| $a_6 = -1.695$ | $a_6 = 1.015$ |

Results in Table 1 were used along with their PY values to compute the C coefficients, using the least square fit equations, equation (40) and (41). Values of C's of $P^*$ are shown in Table 4.

Table 4

Coefficients of P* for Least Square Fit Equation at T* = 3.3333

| n* | C1 | C2 | C3 | C4 | C5 |
|---|---|---|---|---|---|
| 0.85 | 4.28449 | 9.63534 | -1.94971 | -9.25845 | -8.50752 |
| 0.65 | 1.13358 | 1.42599 | -0.383516 | -0.783295 | -0.989399 |

Values of C's in Table 4, together with "exact" values in Table 3 are used to calculate b2 and b3, choosing first the value of b2 and then calculating the corresponding value of b3 to give the correct P*. The results are found in Table 5.

Table 5

Values of b2 and b3 to Give Correct P* at T* = 3.3333

|  | P* |  |
|---|---|---|
| n* | b2 | b3 |
| 0.85 | -0.50 | 0.278 |
|  | -0.45 | 0.256 |
|  | -0.40 | 0.234 |
|  | -0.35 | 0.212 |
|  | -0.30 | 0.190 |
|  | -0.25 | 0.168 |
|  | -0.20 | 0.145 |
|  | -0.15 | 0.123 |
|  | -0.10 | 0.101 |

Table 5--Continued

|  | P* |  |
|---|---|---|
| n* | b2 | b3 |
| 0.85 | 0 | 0.057 |
|  | 0.05 | 0.035 |
|  | 0.10 | 0.013 |
|  | 0.15 | -0.01 |
|  | 0.20 | -0.032 |
|  | 0.25 | -0.054 |
|  | 0.30 | -0.076 |
|  | 0.35 | -0.098 |
|  | 0.40 | -0.120 |
|  | 0.45 | -0.142 |
|  | 0.50 | -0.165 |
| 0.65 | -0.50 | 0.347 |
|  | -0.45 | 0.304 |
|  | -0.40 | 0.262 |
|  | -0.35 | 0.221 |
|  | -0.30 | 0.18 |
|  | -0.25 | 0.138 |
|  | -0.20 | 0.098 |
|  | -0.15 | 0.057 |
|  | -0.10 | 0.173 |
|  | -0.05 | -0.022 |
|  | 0 | -0.062 |

Table 5--Continued

|  | P* |  |
|---|---|---|
| n* | b2 | b3 |
| 0.65 | 0.05 | -0.101 |
|  | 0.10 | -0.14 |
|  | 0.15 | -0.178 |
|  | 0.20 | -0.216 |
|  | 0.25 | -0.254 |
|  | 0.30 | -0.292 |
|  | 0.35 | -0.33 |
|  | 0.40 | -0.467 |
|  | 0.45 | -0.404 |
|  | 0.50 | -0.440 |

A graph is plotted for $b_2$ versus $b_3$ for each density n*= 0.85 and n*= 0.65. As shown in Figure 6, the lines cross each other at the value of $b_2$ = -0.33 and $b_3$ = 0.19 which gives the best fit parameter of equation T at this isotherm. With these new parameters, the integral equation is again solved for a new value of density and the values of P* and U* are redetermined. Results are shown in Table 6.

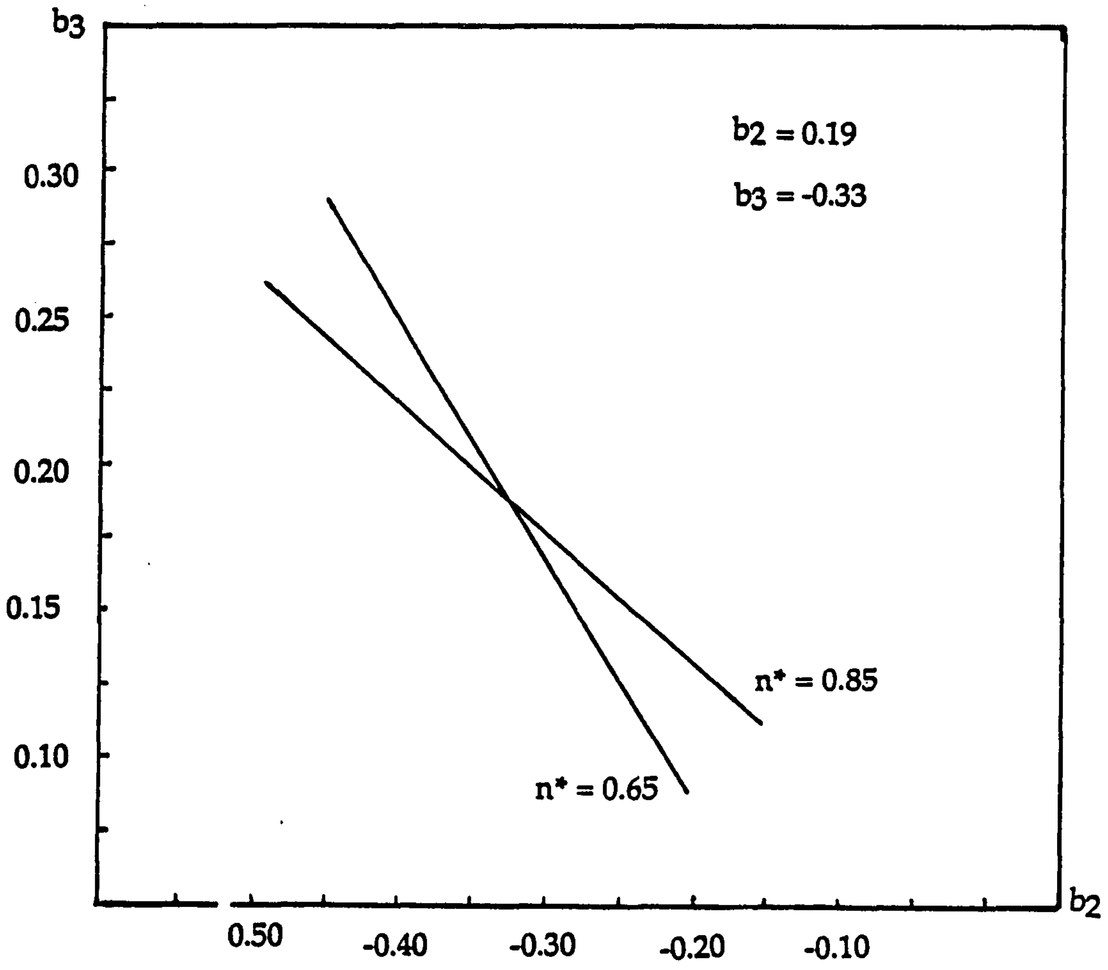

Figure 6. b2 Versus b3 of P* at T* = 3.3333.

Table 6

Results of New Best Fit Parameter at $T^*=3.3333$

| $n^*$ | $P^*$ | $U^*$ |
|---|---|---|
| 0.001 | 1.0004 | 0.9987 |
| 0.10 | 1.0557 | 0.8662 |
| 0.30 | 1.3465 | 0.5924 |
| 0.50 | 2.1318 | 0.2958 |
| 0.70 | 4.1987 | -0.0062 |
| 0.80 | 6.385 | -0.1358 |
| 0.85 | 7.9789 | -0.1899 |

Before a comparison is made, these new $P^*$ and $U^*$ values are used with equations (42) and (43) to get the best values for the interpolation coefficients. Results are shown in Tables 7 and 8 where comparisons are made with "exact" results and equation C results. A graph is drawn in Figure 7 and 8.

Table 7

Comparison of The "Exact" and Equation C Results with The Best Fit of Equation T for $P^*$ and $U^*$

|  | $n^*$ | Equation T | Equation C | "Exact" |
|---|---|---|---|---|
| $P^*$ | 0.05 | 1.0223 | 1.0223 | 1.0223 |
|  | 0.10 | 1.0553 | 1.0553 | 1.0553 |

Table 7--Continued

| | n* | Equation T | Equation C | "Exact" |
|---|---|---|---|---|
| P* | 0.15 | 1.1010 | 1.1016 | 1.1015 |
| | 0.20 | 1.162 | 1.165 | 1.164 |
| | 0.25 | 1.243 | 1.249 | 1.249 |
| | 0.30 | 1.346 | 1.360 | 1.366 |
| | 0.35 | 1.48 | 1.506 | - |
| | 0.40 | 1.648 | 1.694 | 1.611 |
| | 0.45 | 1.861 | 1.936 | 1.845 |
| | 0.50 | 2.131 | 2.25 | 2.127 |
| | 0.55 | 2.473 | 2.63 | 2.480 |
| | 0.60 | - | 3.12 | 2.925 |
| | 0.65 | - | 3.72 | 3.488 |
| | 0.70 | 4.198 | 4.46 | 4.20 |
| | 0.75 | 5.142 | 5.4 | 5.10 |
| | 0.80 | 6.384 | - | 6.237 |
| | 0.85 | 7.978 | | 7.666 |
| U* | 0.05 | 0.93305 | 0.93304 | 0.93309 |
| | 0.10 | 0.86621 | 0.86620 | 0.86618 |
| | 0.15 | 0.79914 | 0.79905 | 0.79888 |
| | 0.20 | 0.7314 | 0.7312 | 0.731 |
| | 0.25 | 0.6626 | 0.6625 | 0.6625 |
| | 0.30 | 0.5924 | 0.5923 | 0.5932 |
| | 0.35 | 0.5207 | 0.5207 | 0.5232 |

Table 7--Continued

| $n^*$ | Equation T | Equation C | "Exact" |
|---|---|---|---|
| 0.40 | 0.4472 | 0.4476 | 0.4524 |
| 0.45 | 0.3722 | 0.3731 | 0.3084 |
| 0.50 | 0.2958 | 0.2977 | 0.2352 |
| 0.55 | 0.2187 | 0.2214 | 0.1611 |
| 0.60 | 0.1418 | 0.1462 | 0.0862 |
| 0.65 | 0.06634 | 0.0721 | 0.0106 |
| 0.70 | -0.0062 | 0.0004 | -0.065 |
| 0.75 | -0.0741 | -0.067 | |
| 0.80 | -0.1357 | | |
| 0.85 | -0.18987 | | |
| 0.90 | -0.23544 | | |
| 0.95 | -0.2721 | | |

Pade' Coefficients of Equation T

| $P^*$ | $U^*$ |
|---|---|
| $a_1 = -2.09106$ | $a_1 = -2.37036$ |
| $a_2 = 2.78619$ | $a_2 = 1.6803$ |
| $a_3 = -1.87646$ | $a_3 = -0.487793$ |
| $a_4 = -2.44513$ | $a_4 = -1.0274$ |
| $a_5 = 1.9071$ | $a_5 = 0.192993$ |
| $a_6 = -0.47073$ | $a_6 = 0.427292$ |

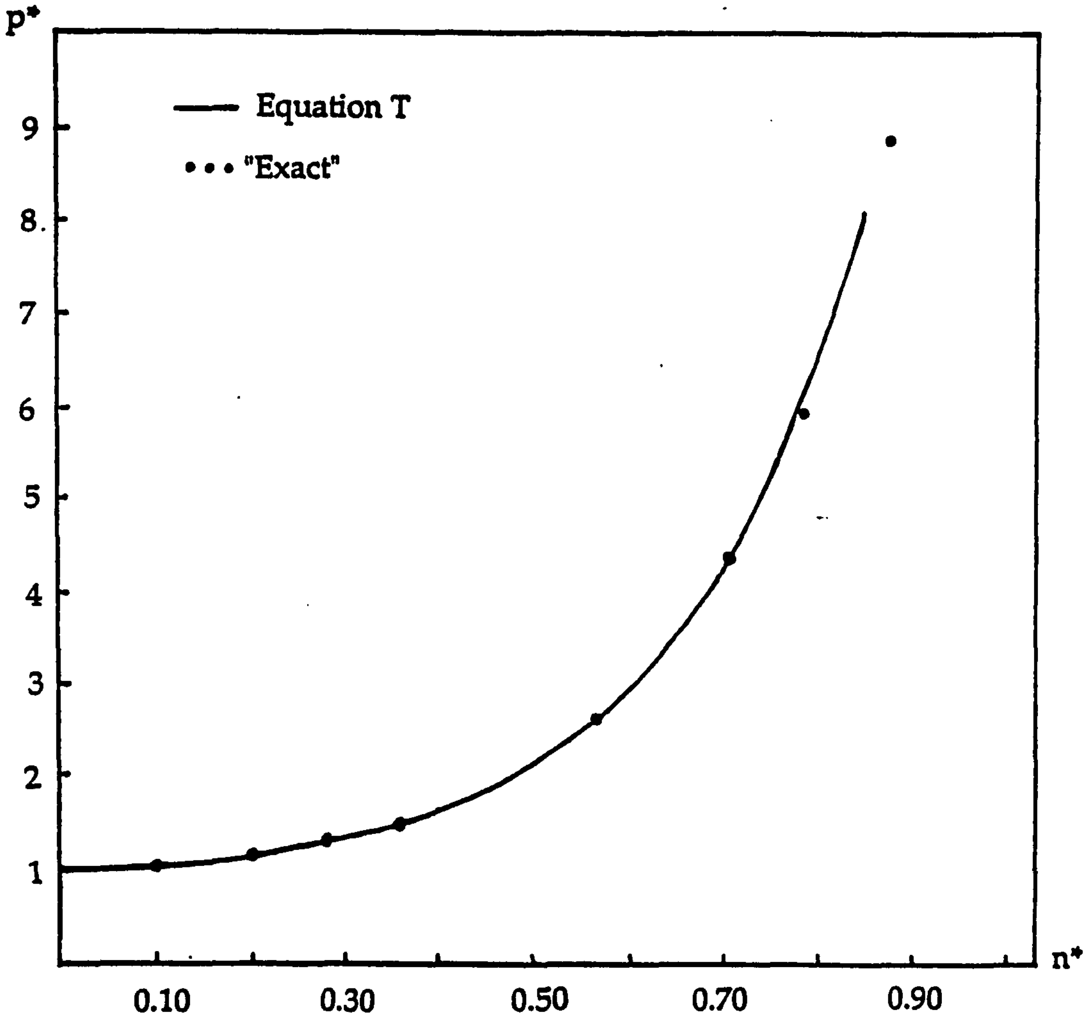

Figure 7. P* Versus n* at T* = 3.3333.

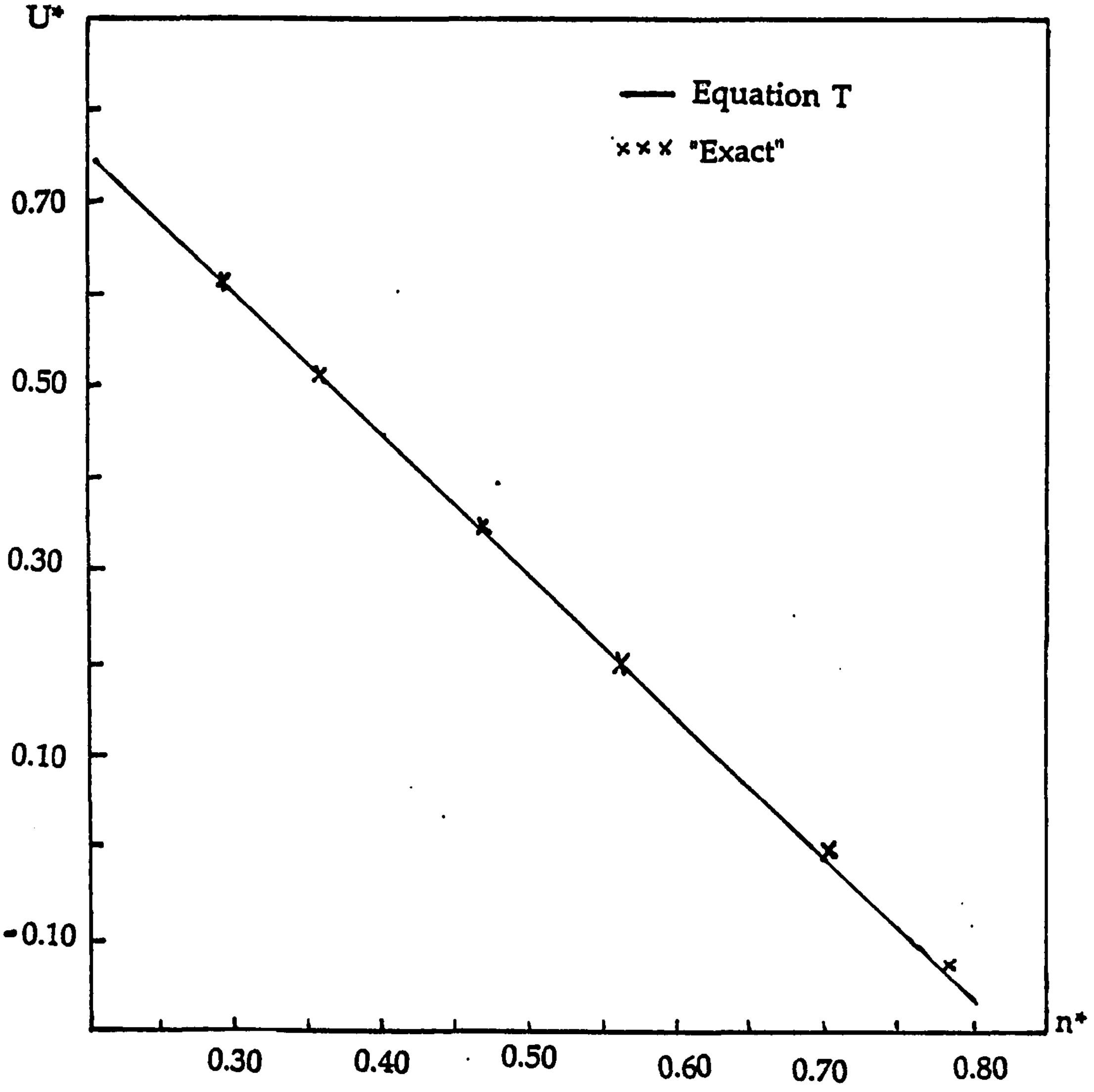

Figure 8. U* Versus n* at T* = 3.3333

## Results in Low Temperature Gas Region .

The next temperatures studied are low ranged temperatures $T^* = 2.6$, $T^* = 1.8$ and $T^* = 1.4$. Table 8 show results of solving integral equation T for several sets of parameters for densities of 0.85 and 0.65. New sets of parameters are used for convenience to get good convergence. Again, only 297 point solutions are listed here.

Table 8

$P^*$ and $U^*$ Using Equation T at $T^* = 2.6$, 1.8 and 1.4

| $T^*$ | b2 | b3 | $n^*$ | $P^*$ | $U^*$ |
|---|---|---|---|---|---|
| | 0 | 0 | 0.85 | 6.908 | -0.532 |
| | -0.7 | 0.60 | | 8.993 | -0.517 |
| | -0.8 | 0.65 | | 9.078 | -0.521 |
| | -0.85 | 0.40 | | 8.532 | -0.533 |
| | -0.8 | 0.45 | | 8.62 | -0.527 |
| | -0.7 | 0.40 | | 8.358 | -0.526 |
| | -0.85 | 0.60 | | 9.131 | -0.520 |
| | -0.7 | 0.60 | 0.65 | 3.293 | -0.206 |
| | -0.8 | 0.65 | | 3.264 | -0.208 |
| | -0.85 | 0.40 | | 2.828 | -0.215 |
| | -0.8 | 0.45 | | 2.989 | -0.212 |
| | -0.7 | 0.40 | | 3.031 | -0.21 |
| | -0.85 | 0.60 | | 3.147 | -0.210 |

Table 8--Continued

| T* | b2 | b3 | n* | P* | U* |
|---|---|---|---|---|---|
| 1.8 | 0 | 0 | 0.85 | 6.418 | -1.225 |
| | -0.225 | 0.15 | | 6.587 | -1.213 |
| | -0.15 | 0.1 | | 6.522 | -1.216 |
| | -0.4 | 0.2 | | 6.374 | -1.21 |
| | -0.3 | 0.1 | | 5.976 | -1.216 |
| | -0.6 | 0.2 | | 5.750 | -1.225 |
| | 0.1175 | 0.0092 | | 6.683 | -1.224 |
| | 0 | 0 | 0.65 | 2.729 | -0.763 |
| | -0.225 | 0.15 | | 2.680 | -0.761 |
| | -0.15 | 0.1 | | 2.577 | -0.765 |
| | -0.4 | 0.2 | | 2.698 | -0.792 |
| | -0.3 | 0.1 | | 2.597 | -0.761 |
| | -0.6 | 0.2 | | 2.445 | -0.762 |
| | 0.1175 | 0.0092 | | 2.796 | -0.764 |
| 1.4 | 0 | 0 | 0.85 | 5.949 | -1.875 |
| | 0.1175 | 0.0092 | | 6.316 | -1.885 |
| | 0.05 | -0.2 | | 5.111 | -1.9 |
| | 0.15 | -0.1 | | 6.023 | -1.900 |
| | 0.2 | -0.1 | | 6.185 | -1.908 |
| | 0.15 | -0.2 | | 5.557 | -1.915 |
| | 0.2 | -0.2 | | 5.789 | -1.925 |

Table 8--Continued.

| T* | $b_2$ | $b_3$ | n* | P* | U* |
|---|---|---|---|---|---|
| 1.8 | 0 | 0 | 0.65 | 2.22 | -1.299 |
| | 0.1175 | 0.0092 | | 2.242 | -1.304 |
| | 0.2 | -0.1 | | 2.217 | -1.316 |
| | 0.05 | -0.2 | | 2.166 | -1.306 |
| | 0.15 | -0.2 | | 2.034 | -1.317 |
| | 0.15 | -0.1 | | 2.212 | -1.308 |
| | 0.2 | -0.2 | | 2.183 | -1.313 |

"Exact" results used for T* = 2.6, 1.8 and 1.4 are shown in Table 9. Their fitted results are shown in Table 10 along with their Pade' coefficients.

Table 9

"Exact" Results for P* and U* at T* = 2.6, 1.8 and 1.4

| Source | T* | n* | P* | U* |
|---|---|---|---|---|
| Results from Carley and Dotson Integral and pertubation method | 2.6 | 0.001 | 0.997663 | 0.998127 |
| | | 0.05 | 0.99 | 0.91 |
| | | 0.10 | 1.00 | 0.82 |
| | | 0.20 | 1.05 | 0.64 |
| | | 0.25 | 1.10 | 0.55 |

Table 9--Continued

| | T* | n* | P* | U* |
|---|---|---|---|---|
| Results as read from Alder's graph. | 2.6 | 0.2828 | 1.15 | 0.50 |
| | | 0.3536 | 1.27 | 0.35 |
| | | 0.4174 | 1.64 | 0.15 |
| | | 0.5657 | 2.20 | -0.05 |
| | | 0.7071 | 3.94 | -0.30 |
| | | 0.7857 | 5.50 | -0.50 |
| | | 0.8319 | 6.53 | -0.60 |
| | | 0.8839 | 8.20 | -0.65 |
| Results from Carley and Dotson Integral Equation and Pertubation Method. | 1.8 | 0.001 | 0.998402 | 0.996790 |
| | | 0.05 | 0.93 | 0.84 |
| | | 0.10 | 0.87 | 0.69 |
| | | 0.15 | 0.83 | 0.55 |
| | | 0.20 | 0.81 | 0.42 |
| | | 0.25 | 0.80 | 0.29 |
| | | 0.30 | 0.80 | 0.16 |
| | | 0.35 | 0.83 | 0.03 |
| | | 0.40 | 0.89 | -0.11 |
| | | 0.45 | 1.00 | -0.25 |
| Results as read from Alder's graph. | | 0.2828 | 0.80 | 0.20 |
| | | 0.3143 | 0.80 | 0.075 |
| | | 0.3536 | 0.85 | 0 |

Table 9--Continued

| Source | T* | n* | P* | U* |
|---|---|---|---|---|
| Results as read from Alder's graph. | 1.8 | 0.4747 | 1.05 | - 0.25 |
| | | 0.5657 | 1.50 | -0.55 |
| | | 0.7071 | 3.00 | -1.00 |
| | | 0.7857 | 4.60 | -1.15 |
| | | 0.8319 | 5.70 | -1.25 |
| | | 0.8839 | 7.50 | -1.35 |
| Results from Carley and Dotson Integral Equation and Pertubation Method. | 1.4 | 0.001 | 0.998402 | 0.99679 |
| | | 0.05 | 0.86 | 0.84 |
| | | 0.10 | 0.74 | 0.69 |
| | | 0.15 | 0.64 | 0.55 |
| | | 0.20 | 0.58 | 0.42 |
| | | 0.25 | 0.53 | 0.29 |
| Results as read from Alder's graph. | | 0.2828 | 0.50 | -0.07 |
| | | 0.3143 | 0.45 | -0.20 |
| | | 0.3536 | 0.45 | -0.35 |
| | | 0.4714 | 0.50 | -0.67 |
| | | 0.5657 | 0.75 | -1.00 |
| | | 0.7071 | 2.20 | -1.50 |
| | | 0.7857 | 3.70 | -1.80 |
| | | 0.8319 | 5.00 | -1.95 |
| | | 0.8839 | 6.80 | -2.05 |

Table 10

Fitted "Exact" Results for T* = 2.6, 1.8, 1.4

| T* | n* | P* | U* |
|---|---|---|---|
| 2.6 | 0.05 | 0.996 | 0.901 |
| | 0.10 | 0.995 | 0.827 |
| | 0.15 | 1.011 | 0.73 |
| | 0.20 | 1.044 | 0.636 |
| | 0.25 | 1.099 | 0.543 |
| | 0.30 | 1.183 | 0.450 |
| | 0.35 | 1.311 | 0.357 |
| | 0.40 | 1.520 | 0.263 |
| | 0.45 | 2.393 | 0.169 |
| | 0.50 | 1.593 | 0.075 |
| | 0.55 | 2.059 | -0.020 |
| | 0.60 | 2.532 | -0.116 |
| | 0.65 | 3.111 | -0.218 |
| | 0.70 | 3.833 | -0.281 |
| | 0.75 | 4.732 | -0.391 |
| | 0.80 | 5.837 | -0.488 |
| | 0.85 | 7.167 | -0.585 |
| | 0.90 | 8.722 | -0.681 |
| | 0.95 | 10.47 | -0.777 |
| | 1.00 | 12.35 | -0.874 |

Table 10--Continued

| T* | n* | P* | U* |
|---|---|---|---|
| 1.8 | 0.05 | 0.947 | 0.843 |
| | 0.10 | 0.898 | 0.694 |
| | 0.15 | 0.856 | 0.55 |
| | 0.20 | 0.824 | 0.410 |
| | 0.25 | 0.804 | 0.274 |
| | 0.30 | 0.80 | 0.141 |
| | 0.35 | 0.851 | 0.009 |
| | 0.40 | 0.895 | -0.121 |
| | 0.45 | 0.946 | -0.250 |
| | 0.50 | 1.16 | -0.379 |
| | 0.55 | 1.403 | -0.509 |
| | 0.60 | 1.752 | -0.641 |
| | 0.65 | 2.239 | -0.783 |
| | 0.70 | 2.901 | -1.207 |
| | 0.75 | 3.783 | - |
| | 0.80 | 4.926 | -1.22 |
| | 0.85 | 6.360 | -1.258 |
| | 0.90 | 8.085 | -1.393 |
| | 0.95 | 10.05 | -1.529 |
| | 1.00 | 12.12 | -1.665 |
| 1.4 | 0.05 | 0.892 | 0.764 |
| | 0.10 | 0.787 | 0.540 |
| | 0.15 | 0.689 | 0.33 |

Table 10--Continued

| T* | n* | P* | U* |
|---|---|---|---|
| 1.4 | 0.20 | 0.599 | -0.35 |
| | 0.25 | 0.522 | -0.426 |
| | 0.30 | 0.463 | - |
| | 0.35 | 0.428 | - |
| | 0.40 | 0.426 | -0.472 |
| | 0.45 | 0.467 | -0.611 |
| | 0.50 | 0.563 | -0.769 |
| | 0.55 | 0.718 | -0.944 |
| | 0.60 | 1.147 | -1.124 |
| | 0.65 | 1.503 | -1.303 |
| | 0.70 | 2.097 | -1.476 |
| | 0.75 | 2.929 | -1.642 |
| | 0.80 | 4.056 | -1.8 |
| | 0.85 | 5.546 | -1.951 |
| | 0.90 | 7.469 | -2.1 |
| | 0.95 | 9.878 | -2.235 |
| | 1.00 | 12.79 | -2.369 |

Table 10--Continued

Pade' Coefficients for $P^*$

| Coefficients | $T^* = 2.6$ | $T^* = 1.8$ | $T^* = 1.4$ |
|---|---|---|---|
| $a_1$ | -3.95329 | -5.724 | -5.40844 |
| $a_2$ | 6.44708 | 11.3766 | 10.6507 |
| $a_3$ | -5.57169 | -9.50623 | -7.40751 |
| $a_4$ | -3.72132 | -4.62341 | -3.22023 |
| $a_5$ | 4.05959 | 5.68353 | 3.21404 |
| $a_6$ | -1.50414 | -2.29556 | -1.08495 |

Pade' Coefficients For $U^*$

| Coefficients | $T^* = 2.6$ | $T^* = 1.8$ | $T^* = 1.4$ |
|---|---|---|---|
| $a_1$ | -17.1846 | -3.51492 | -8.16153 |
| $a_2$ | 48.7258 | 0.912704 | 21.3391 |
| $a_3$ | -37.6429 | 2.91196 | -19.8052 |
| $a_4$ | -15.3123 | -0.303127 | -3.32219 |
| $a_5$ | 20.6739 | -1.81646 | 2.89548 |
| $a_6$ | -0.523841 | 0.332932 | 1.80226 |

Again, at this point the least square fit equation are used to calculate C's for each corresponding results in Table 8. Results are shown in Table 11.

## Table 11

## Coefficients of The Least Square Fit Equation for P*

$T^* = 2.6$

| $n^*$ | $C_1$ | $C_2$ | $C_3$ | $C_4$ | $C_5$ |
|---|---|---|---|---|---|
| 0.85 | 6.51807 | 13.0166 | 5.4668 | -8.45703 | 1.9043 |
| 0.65 | 0.945435 | 1.00952 | -0.788452 | -1.11749 | -2.0144 |

$T^* = 1.8$

| $n^*$ | $C_1$ | $C_2$ | $C_3$ | $C_4$ | $C_5$ |
|---|---|---|---|---|---|
| 0.85 | 3.6217 | 5.88789 | -0.971191 | -3.55859 | -6.83984 |
| 0.65 | 0.564087 | 0.574219 | -0.340332 | -0.679688 | -0.764094 |

$T^* = 1.4$

| $n^*$ | $C_1$ | $C_2$ | $C_3$ | $C_4$ | $C_5$ |
|---|---|---|---|---|---|
| 0.85 | 3.16312 | 4.15126 | -2.38828 | -6.16533 | -8.7646 |
| 0.65 | 0.190654 | 0.286202 | -0.222214 | -0.108007 | -.117786 |

Values of C's in Table 11, together with values of pressure in Table 10 are used to calculate $b_2$ and $b_3$ choosing first the value $b_2$ and then calculating the value of $b_3$ for each corresponding temperature. The results can be found in Table 12.

Table 12

Values of $b_2$ and $b_3$ to Give Correct P* for T* = 2.6, 1.8 and 1.4

| T* | b2 | b3 | |
|---|---|---|---|
| | | n* = 0.85 | n* = 0.65 |
| 2.6 | -0.50 | 0.209 | 0.288 |
| | -0.45 | 0.199 | 0.146 |
| | -0.40 | 0.187 | 0.203 |
| | -0.35 | 0.172 | 0.160 |
| | -0.30 | 0.155 | 0.117 |
| | -0.25 | 0.136 | 0.073 |
| | -0.20 | 0.115 | 0.028 |
| | -0.15 | 0.093 | -0.017 |
| | - 0.10 | 0.07 | -0.062 |
| | -0.05 | 0.046 | -0.108 |
| | 0 | 0.20 | -0.154 |
| | 0.05 | 0.006 | -0.200 |
| | 0.10 | -0.033 | -0.247 |
| 1.8 | -0.95 | 0.389 | 0.334 |
| | -0.90 | 0.374 | 0.277 |
| | -0.85 | 0.359 | 0.222 |
| | -0.80 | 0.343 | 0.169 |
| | -0.75 | 0.267 | 0.118 |
| | -0.70 | 0.310 | 0.068 |

Table 12--Continued

| T* | b2 | b3 | |
|---|---|---|---|
| 1.8 | | n* = 0.85 | n* = 0.65 |
| | -0.65 | 0.293 | 0.019 |
| | -0.60 | 0.275 | -0.028 |
| | -0.55 | 0.256 | -0.074 |
| | -0.50 | 0.237 | -0.120 |
| | -0.45 | 0.217 | -0.164 |
| | -0.40 | 0.196 | -0.207 |
| 1.4 | 1.60 | -0.071 | -0.807 |
| | 1.65 | -0.092 | -0.759 |
| | 1.70 | -0.113 | -0.709 |
| | 1.75 | -0.135 | -0.658 |
| | 1.80 | -0.156 | -0.604 |
| | 1.85 | -0.177 | -0.549 |
| | 1.90 | -0.197 | -0.492 |
| | 2.00 | -0.218 | -0.434 |
| | 2.05 | -0.259 | -0.311 |
| | 2.10 | -0.280 | -0.246 |
| | 2.15 | -0.300 | -0.180 |
| | 2.20 | -0.320 | -0.110 |
| | 2.25 | -0.340 | -0.0385 |
| | 2.30 | -0.361 | -0.035 |

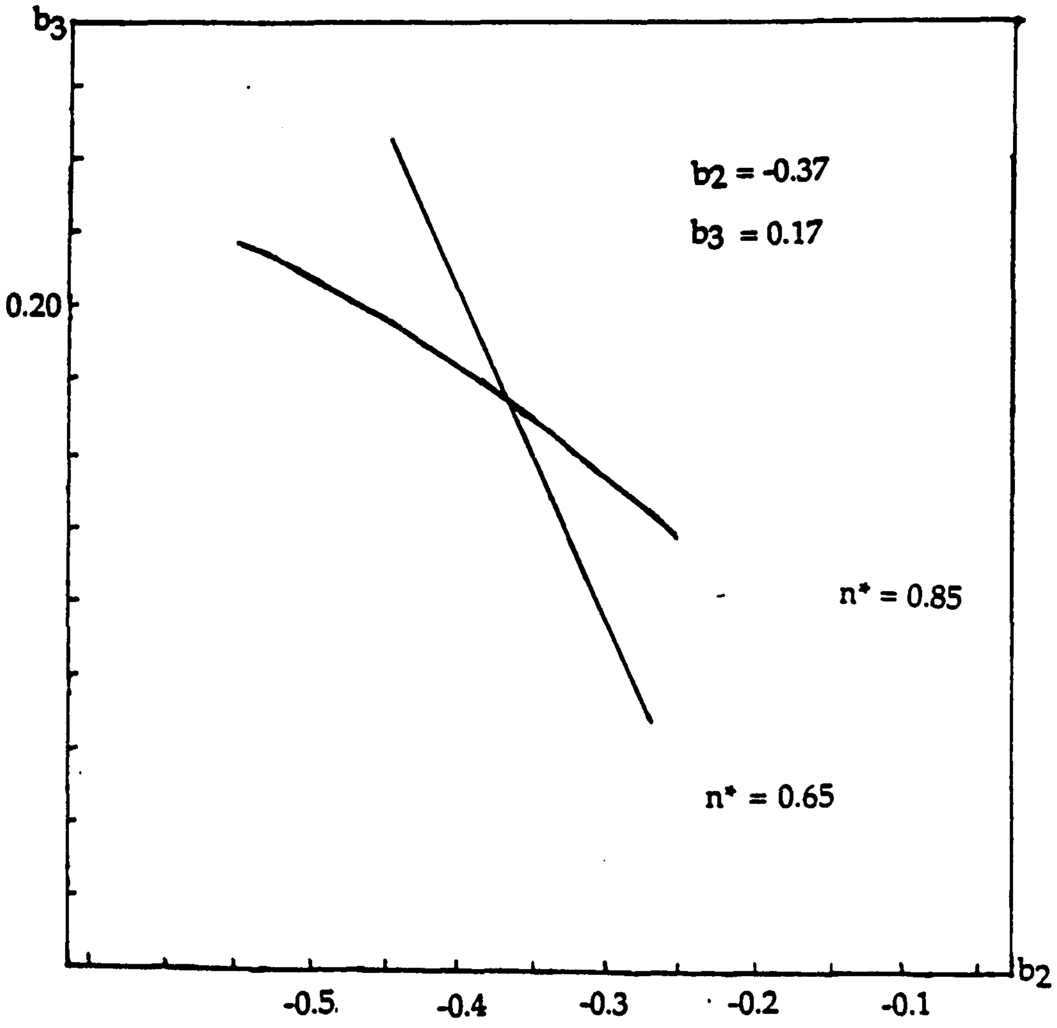

Figure 9. b2 Versus b3 of P* at T* = 2.6

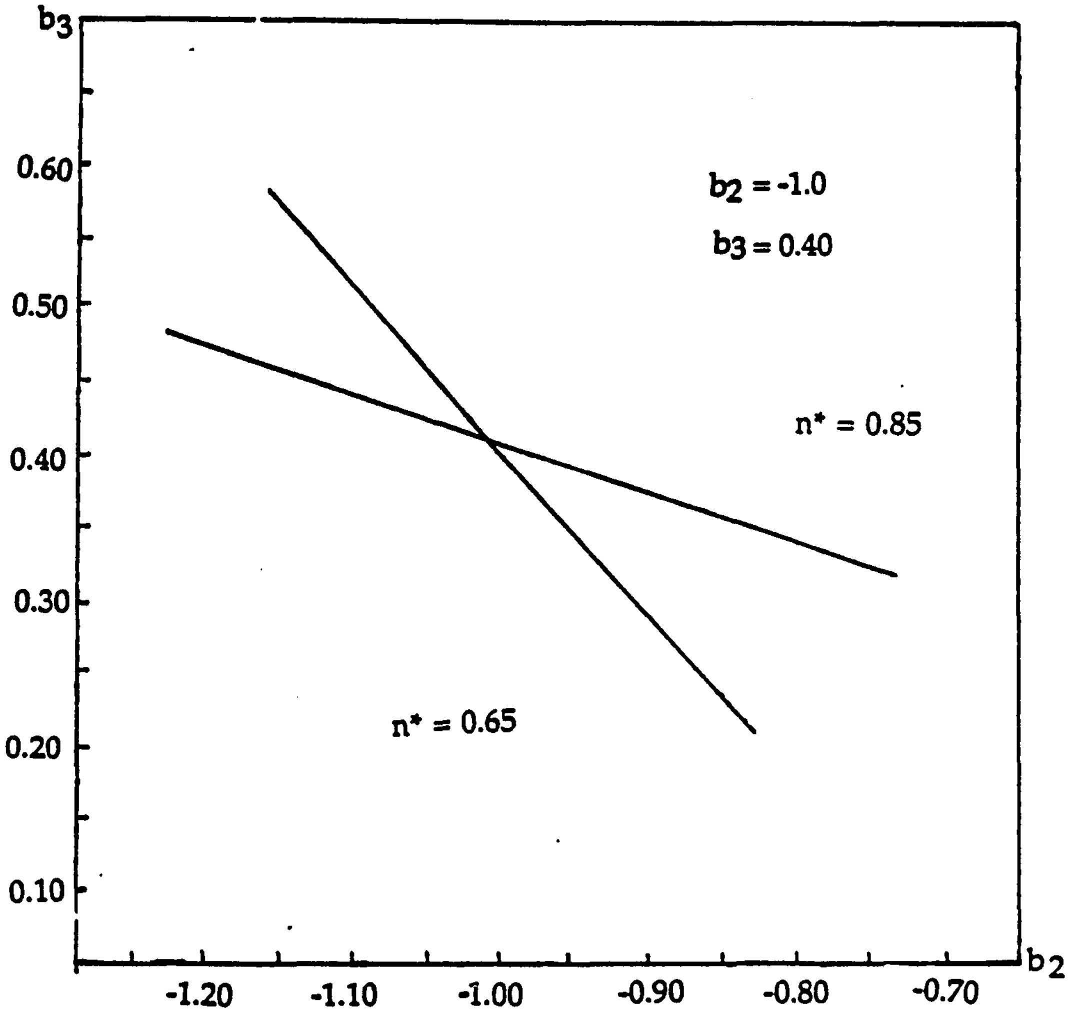

Figure 10 b2 Versus b3 of P* at T* = 1.8

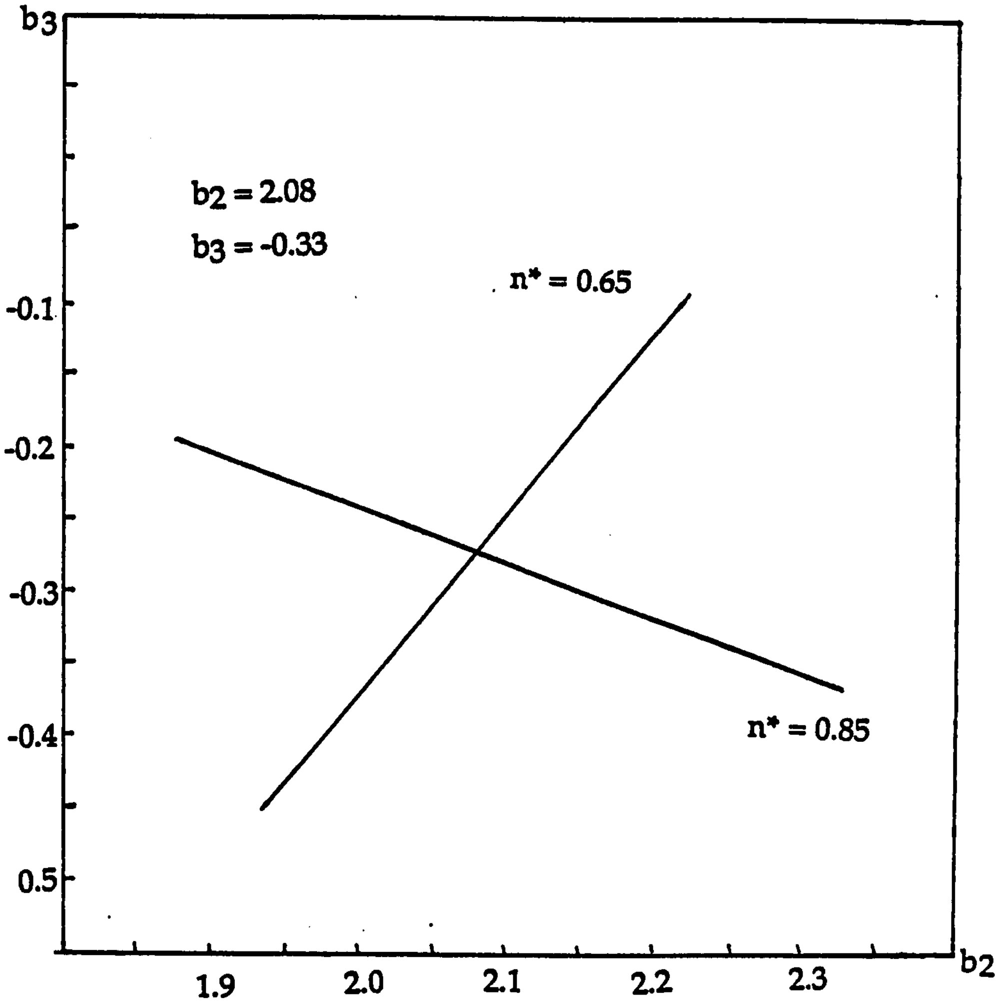

Figure 11. b2 Versus b3 of P* at T* = 1.4.

Graphs are plotted for $b_2$ versus $b_3$ for each temperature. As can be seen from Figures 9, 10 and 11, the lines cross at a point to give the best values of parameters $b_2$ and $b_3$ for equation T. With these new parameters, equation T is again solved for new values of densities. As noted, when the density increases and when the tempetartue decreases good convergence is very hard to obtain. That is why only values of $P^*$ and $U^*$ at temperature $T^* = 2.6$ and 1.8 can be obtained since they give convergence. At temperature $T^* = 1.4$ no convergence can be found. Results for these two temperatures are listed in Table 13 and their fitted values with Pade' coefficients are in Table 14.

Table 13

Result Using Best Fit Parameters of Equation T at $T^* = 2.6$ and 1.8

| $T^*$ | $n^*$ | $P^*$ | $U^*$ |
|---|---|---|---|
| 2.6 | 0.001 | 1 | 0.998 |
| | 0.10 | 0.976 | 0.813 |
| | 0.30 | 1.184 | 0.459 |
| | 0.50 | 1.876 | 0.037 |
| | 0.65 | 3.096 | -0.206 |
| | 0.75 | 4.601 | -0.384 |
| | 0.85 | 7.205 | -0.530 |
| 1.8 | 0.001 | 0.998 | 0.997 |
| | 0.10 | 0.873 | 0.694 |

Table 13--Continued

| $T^*$ | $n^*$ | $P^*$ | $U^*$ |
|---|---|---|---|
| | 0.25 | 0.838 | 0.291 |
| | 0.45 | 1.204 | -0.226 |
| | 0.60 | 1.904 | -0.63 |
| | 0.70 | 2.642 | -1.022 |
| | 0.75 | 3.419 | -1.215 |
| | 0.85 | 7.108 | -0.897 |

$T^* = 2.6$ $b_2 = -0.37$ $b_3 = 0.17$

$T^* = 1.8$ $b_3 = -1.0$ $b_3 = 0.40$

Table 14

Results From Equation T Using Pade' Equation at $T^* = 2.6$ and 1.8

| $T^*$ | $n^*$ | $P^*$ | $U^*$ |
|---|---|---|---|
| 2.6 | 0.05 | 0.993 | 0.907 |
| | 0.10 | 0.998 | 0.814 |
| | 0.15 | 1.017 | 0.723 |
| | 0.20 | 1.052 | 0.632 |
| | 0.25 | 1.107 | 0.544 |
| | 0.30 | 1.185 | 0.460 |
| | 0.35 | 1.290 | 0.384 |

Table 14--Continued

| T* | n* | P* | U* |
|---|---|---|---|
| 2.6 | 0.40 | 1.452 | 0.278 |
| | 0.45 | 1.632 | 0.157 |
| | 0.50 | 1.874 | 0.038 |
| | 0.55 | 2.186 | -0.083 |
| | 0.60 | 2.584 | -0.121 |
| | 0.65 | 3.094 | -0.206 |
| | 0.70 | 3.75 | -0.293 |
| | 0.75 | 4.6 | -0.384 |
| | 0.80 | 5.715 | -0.681 |
| | 0.85 | 7.202 | -0.530 |
| | 0.90 | 9.234 | -0.622 |
| | 0.95 | 12.103 | -0.708 |
| 1.8 | 0.05 | 0.927 | 0.844 |
| | 0.10 | 0.872 | 0.697 |
| | 0.15 | 0.837 | 0.557 |
| | 0.20 | 0.824 | 0.422 |
| | 0.25 | 0.838 | 0.291 |
| | 0.30 | 0.88 | 0.161 |
| | 0.35 | 0.953 | 0.033 |
| | 0.40 | 1.06 | -0.096 |
| | 0.45 | 1.20 | -0.226 |

Table 14--Continued

| $T^*$ | $n^*$ | $P^*$ | $U^*$ |
|---|---|---|---|
| 1.8 | 0.50 | 1.388 | -0.358 |
| | 0.55 | 1.618 | -0.492 |
| | 0.60 | 1.904 | -0.629 |
| | 0.65 | 2.266 | -0.765 |
| | 0.70 | 2.741 | -0.898 |
| | 0.75 | 3.420 | -1.021 |
| | 0.80 | 4.544 | -1.13 |
| | 0.85 | 7.109 | -1.21 |
| | 0.90 | 24.14 | -1.27 |

Pade' Coefficients For $P^*$ and $U^*$

| | $P^*$ | | $U^*$ | |
|---|---|---|---|---|
| Coefficients | $T^* = 2.6$ | $T^* = 1.8$ | $T^* = 2.6$ | $T^* = 1.8$ |
| $a_1$ | -3.99097 | -3.38319 | -5.4253 | -4.04749 |
| $a_2$ | 6.07947 | 7.27675 | 9.53632 | 4.11527 |
| $a_3$ | -6.46582 | -4.64153 | -5.3922 | -1.53251 |
| $a_4$ | -3.75262 | -1.78225 | -3.55185 | -0.835613 |
| $a_5$ | 3.25311 | 1.60823 | 2.73677 | -0.689926 |
| $a_6$ | -0.70713 | -0.93189 | 0.169372 | 0.887224 |

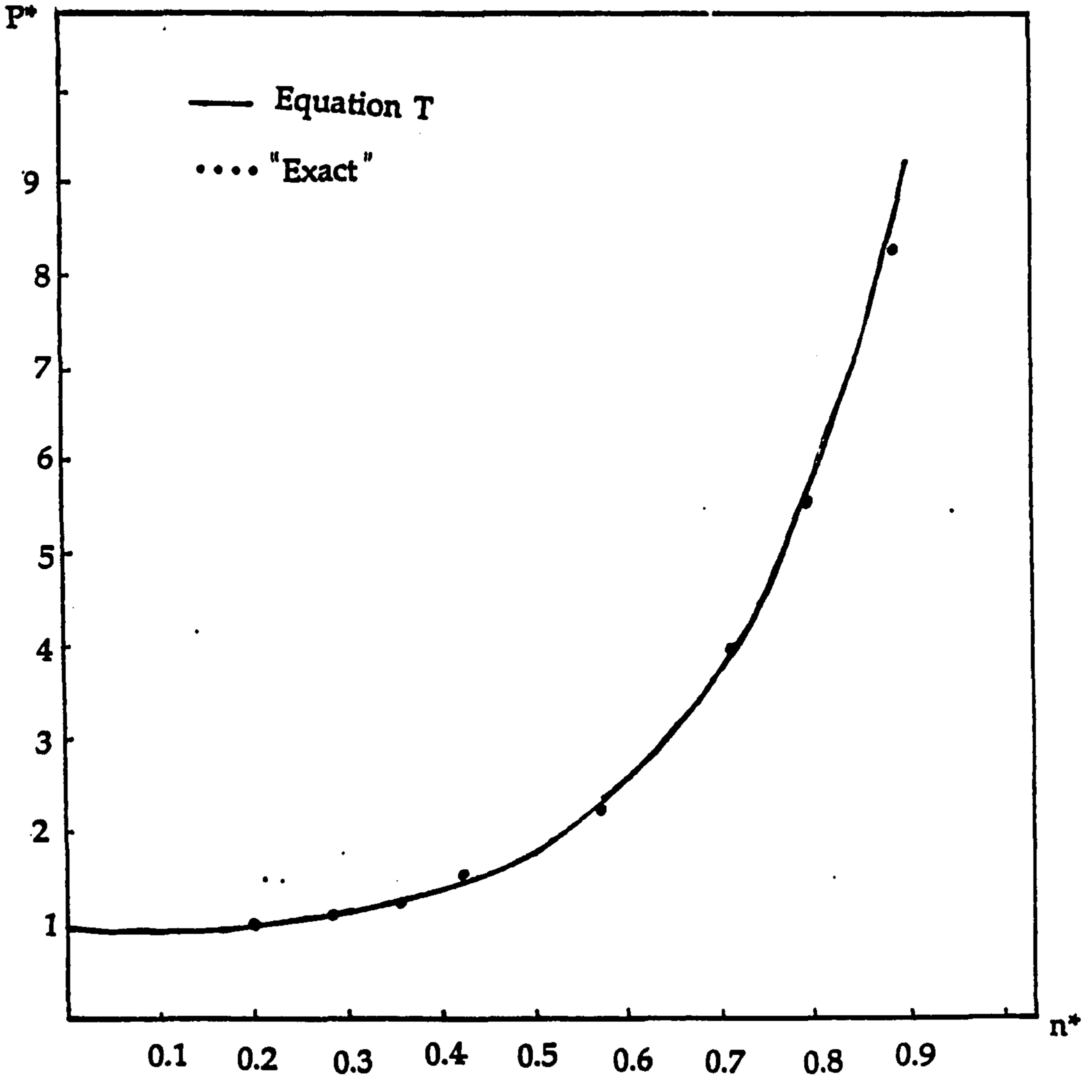

Figure 12. P* Versus n* at T* = 2.6

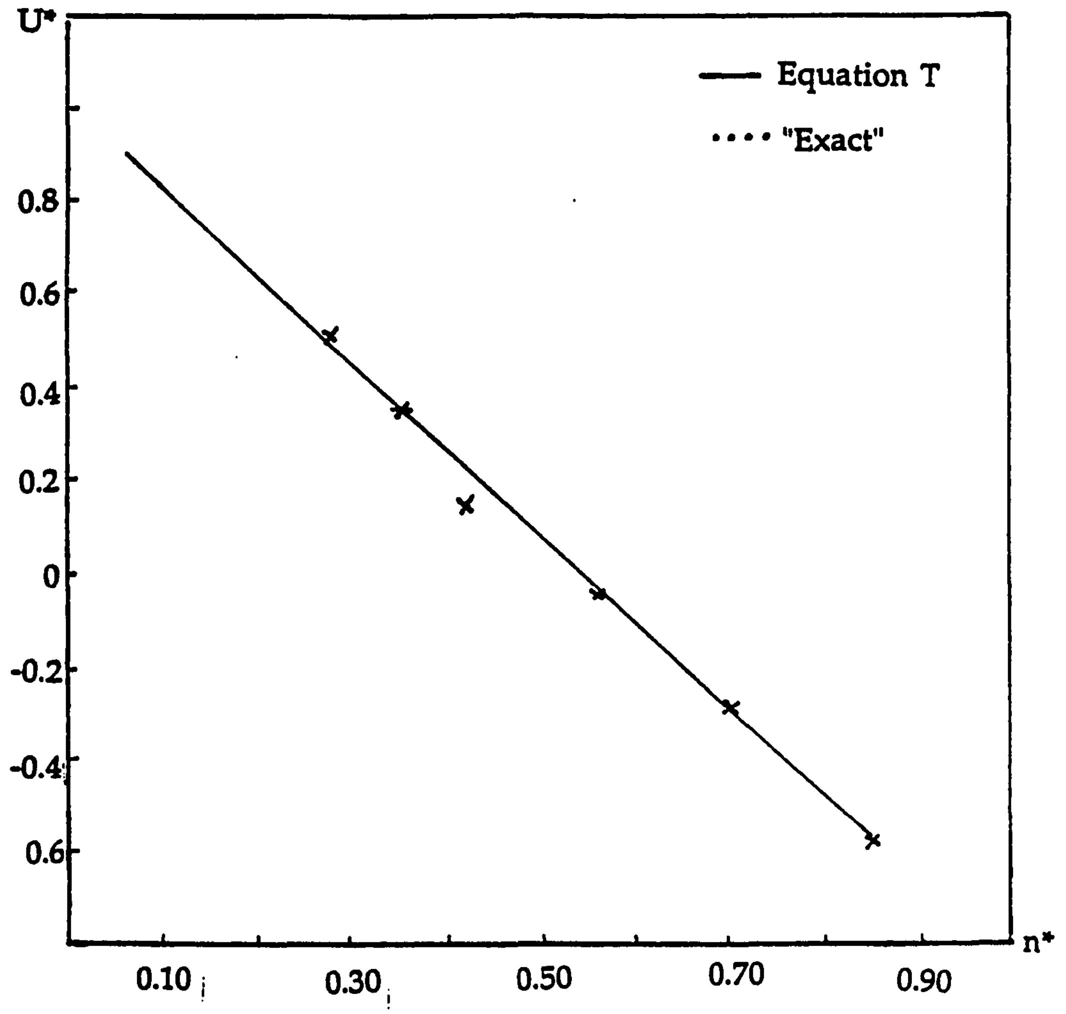

Figure 13. U* Versus n* at T* = 2.6

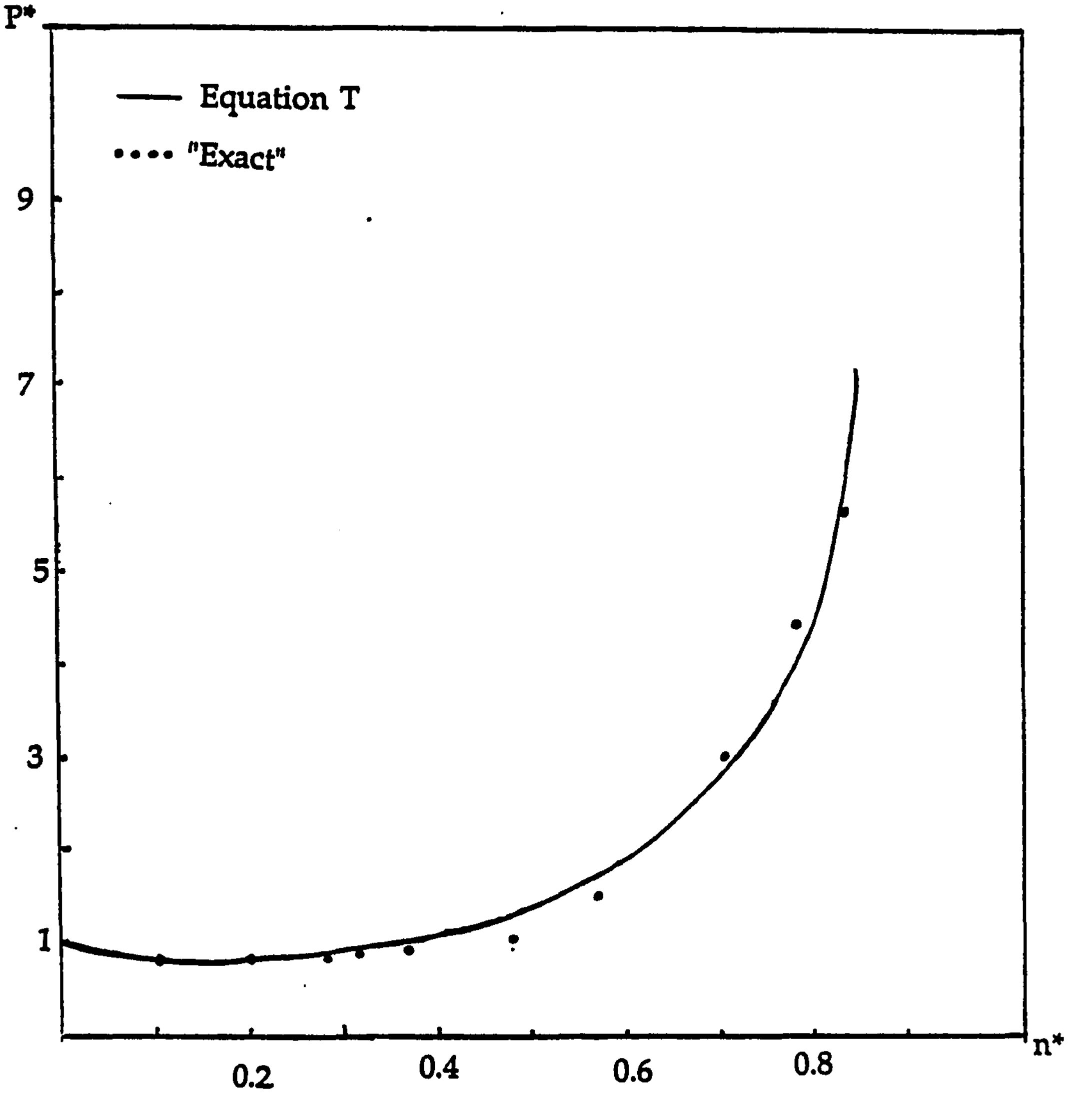

Figure 14. P* Versus n* at T* = 1.8

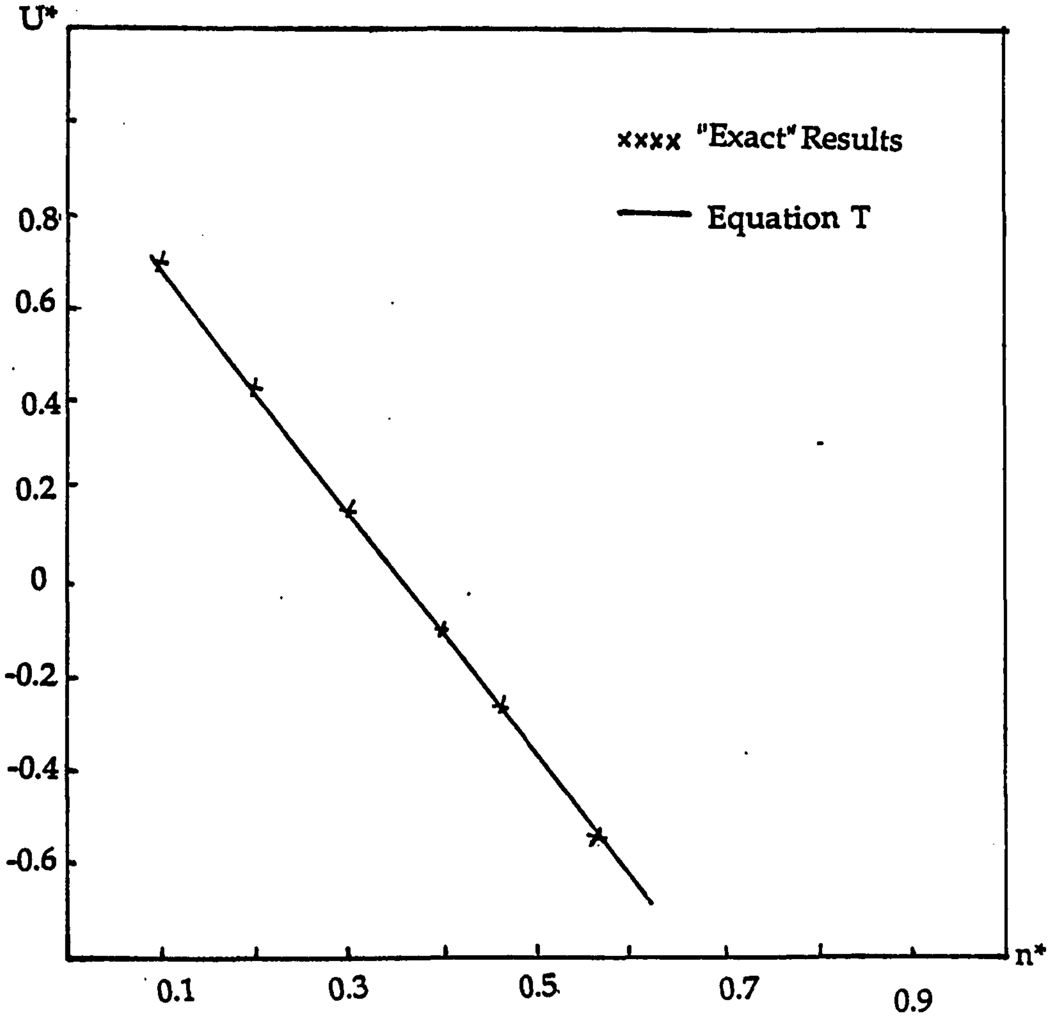

Figure 15. U* Versus n* at T* = 1.8

## Results in High Temperature Gas Region

We next study the high temperature in the gas region, at T* = 6.11, T* = 10 and T* = 20. The method used is the same as for lower temperatures. Results are shown in the following tables. Graphs are again plotted to compare with the "exact" values.

Table 15

Results of P* and U* Using Equation T at T* = 6.11, 10 and 20

| T* | $b_2$ | $b_3$ | n* | P* | U* |
|---|---|---|---|---|---|
| 6.11 | 0 | 0 | 0.85 | 7.536 | 0.353 |
| | 0.1175 | 0.0092 | | 8.224 | 0.356 |
| | 0.5 | 0.1667 | | 10.04 | 0.361 |
| | 0.2 | 0.4 | | 10.42 | 0.362 |
| | -0.25 | 0.3 | | 9.615 | 0.358 |
| | -0.1 | 0.5 | | 10.48 | 0.362 |
| | 0.4 | -0.1 | | 8.241 | 0.357 |
| | 0 | 0 | 0.65 | 4.052 | 0.499 |
| | 0.1175 | 0.0092 | | 4.237 | 0.501 |
| | 0.2 | 0.4 | | 4.82 | 0.504 |
| | -0.25 | 0.3 | | 4.349 | 0.5 |
| | -0.1 | 0.5 | | 4.731 | 0.502 |
| | 0.4 | -0.1 | | 4.388 | 0.503 |
| | 0.5 | 0.1667 | | 4.797 | 0.505 |

Table 15--Continued

| T* | $b_2$ | $b_3$ | n* | P* | U* |
|---|---|---|---|---|---|
| 10 | 0 | 0 | 0.85 | 7.719 | 0.605 |
| | 0.1175 | 0.0092 | | 8.452 | 0.608 |
| | 0.2 | 0.4 | | 10.746 | 0.612 |
| | -0.25 | 0.3 | | 10.00 | 0.609 |
| | -0.1 | 0.5 | | 10.846 | 0.611 |
| | 0.3 | 0.3 | | 10.523 | 0.612 |
| | 0.5 | 0.1667 | | 10.307 | 0.612 |
| | 0 | 0 | 0.65 | 4.279 | 0.696 |
| | 0.11 | 0.0092 | | 4.483 | 0.697 |
| | 0.3 | 0.3 | | 5.089 | 0.7 |
| | 0.2 | 0.4 | | 5.131 | 0.7 |
| | -0.25 | 0.3 | | 4.668 | 0.7 |
| | -0.1 | 0.5 | | 5.062 | 0.699 |
| | 0.5 | 0.1667 | | 5.082 | 0.700 |
| 20 | 0 | 0 | 0.85 | 7.719 | 0.605 |
| | 0.1175 | 0.0092 | | 8.633 | 0.804 |
| | 0.1 | 0.01 | | 8.105 | 0.804 |
| | 0.05 | 0.05 | | 8.89 | 0.804 |
| | 0.1 | 0.04 | | 8.938 | 0.805 |
| | 0.15 | 0.05 | | 9.18 | 0.805 |
| | 0.01 | 0.1667 | | 9.79 | 0.805 |
| | 0 | 0 | 0.65 | 4.46 | 0.849 |

Table 15--Continued

| $T^*$ | $b_2$ | $b_3$ | $n^*$ | $P^*$ | $U^*$ |
|---|---|---|---|---|---|
| 20 | 0.1175 | 0.0092 | 0.65 | 4.678 | 0.85 |
| | 0.1 | 0.01 | | 4.65 | 0.849 |
| | 0.05 | 0.05 | | 4.69 | 0.849 |
| | -0.25 | 0.3 | | 4.927 | 0.849 |
| | 0.1 | 0.5 | | 5.429 | 0.851 |
| | 0.5 | 0.1667 | | 5.306 | 0.851 |

## Table 16

## "Exact" Results Used for $T^*$ = 6.11, 10 and 20

| Source | $T^*$ | $n^*$ | $P^*$ | $U^*$ |
|---|---|---|---|---|
| Monte Carlo results of Rottenberg as read from Alder's graph. | 6.11 | 0.2828 | 1.50 | 0.80 |
| | | 0.3536 | - | 0.75 |
| | | 0.4745 | - | 0.65 |
| | | 0.5657 | 3.28 | 0.55 |
| | | 0.7071 | 5.02 | 0.45 |
| | | 0.7857 | 6.60 | 0.40 |
| | | 0.8319 | 7.70 | 0.33 |
| | | 0.8839 | 9.40 | 0.30 |
| Results from Equation C | 10 | 0.001 | 1.0015734 | 0.9996334 |

Table 16--Continued

| Source | T* | n* | P* | U* |
|---|---|---|---|---|
| Results from equation C | 10 | 0.05 | 1.08424 | 0.98126 |
| | | 0.10 | 1.1814 | 0.96167 |
| | | 0.15 | 1.2943 | 0.94119 |
| | | 0.20 | 1.426 | 0.91979 |
| | | 0.25 | 1.581 | 0.8975 |
| | | 0.30 | 1.764 | 0.8742 |
| | | 0.35 | 1.981 | 0.8502 |
| | | 0.40 | 2.238 | 0.8254 |
| | | 0.45 | 2.544 | 0.8001 |
| | | 0.50 | 2.91 | 0.7743 |
| | | 0.55 | 3.34 | 0.7484 |
| | | 0.60 | 3.86 | 0.7227 |
| | | 0.65 | 4.48 | 0.6973 |
| | | 0.70 | 5.23 | 0.6729 |
| | | 0.75 | 6.1 | 0.6495 |
| | | 0.80 | 7.2 | 0.6279 |
| | | 0.85 | 8.5 | 0.608 |
| Results as read from Alder's graph's. | | 0.8319 | 8.1 | 0.6 |
| | | 0.8839 | 9.5 | 0.6 |
| Results from Equation C | 20 | 0.001 | 1.0018418 | 0.9998156 |
| | | 0.05 | 1.09832 | 0.9103 |

Table 16--Continued

| Source | T* | n* | P* | U* |
|---|---|---|---|---|
| Results from Equation C | 20 | 0.10 | 1.2109 | 0.98153 |
| | | 0.15 | 1.3404 | 0.97150 |
| | | 0.20 | 1.490 | 0.96091 |
| | | 0.25 | 1.663 | 0.9499 |
| | | 0.30 | 1.865 | 0.9382 |
| | | 0.35 | 2.100 | 0.9263 |
| | | 0.40 | 2.376 | 0.1938 |
| | | 0.45 | 2.699 | 0.9011 |
| | | 0.50 | 3.08 | 0.8882 |
| | | 0.55 | 3.53 | 0.8752 |
| | | 0.60 | 4.05 | 0.8623 |
| | | 0.65 | 4.68 | 0.8493 |
| | | 0.70 | 5.42 | 0.8373 |
| | | 0.75 | 6.3 | 0.8254 |
| | | 0.80 | 7.4 | 0.8147 |
| | | 0.85 | 8.7 | 0.804 |

## Table 17

## Interpolated "Exact" Results for P* and U* at T* = 6.11 and Their Corresponding Pade' Coefficients

| n* | P* | U* |
|---|---|---|
| 0.05 | 1.04882 | 0.967123 |
| 0.10 | 1.11854 | 0.933237 |
| 0.15 | 1.21062 | 0.898297 |
| 0.20 | 1.32699 | 0.862255 |
| 0.25 | 1.47009 | 0.825061 |
| 0.30 | 1.64302 | 0.786661 |
| 0.40 | 1.8497 | 0.747001 |
| 0.40 | 2.09509 | 0.706026 |
| 0.45 | 2.38553 | 0.663677 |
| 0.50 | 2.72917 | 0.619896 |
| 0.55 | 3.13664 | 0.574624 |
| 0.60 | 3.62196 | 0.527785 |
| 0.65 | 4.204 | 0.479235 |
| 0.70 | 4.90852 | 0.428214 |
| 0.75 | 5.76996 | 0.360996 |
| 0.80 | 6.86603 | 0.356847 |
| 0.85 | 8.23334 | 0.361222 |
| 0.90 | 10.0333 | 0.120407 |
| 0.95 | 12.482 | 0.10772 |
| 1.00 | 15.9879 | 0.0532304 |

Table 17--continued

| Pade' Coefficients of P* | Pade' Coefficients of U* |
|---|---|
| $a_1 = -0.724881$ | $a_1 = -3.3998$ |
| $a_2 = 2.59592$ | $a_2 = 3.82276$ |
| $a_3 = -4.23454$ | $a_3 = -1.4213$ |
| $a_4 = -1.50023$ | $a_4 = -2.75206$ |
| $a_5 = -0.194393$ | $a_5 = 2.23317$ |
| $a_6 = 0.609337$ | $a_6 = -0.449848$ |

Table 18

Coefficients C's of Least Square Fit Equation at T* = 6.11, 10 and 20

T* = 6.11

| n* | $C_1$ | $C_2$ | $C_3$ | $C_4$ | $C_5$ |
|---|---|---|---|---|---|
| 0.85 | 5.67657 | 13.6122 | -3.9586 | -15.5894 | -13.7615 |
| 0.65 | 1.52907 | 2.39239 | -0.700459 | -1.85059 | -2.23718 |

T* = 10

| n* | $C_1$ | $C_2$ | $C_3$ | $C_4$ | $C_5$ |
|---|---|---|---|---|---|
| 0.85 | 5.35228 | 14.3692 | -3.65118 | -16.5302 | -20.568 |
| 0.65 | 1.58129 | 2.85393 | -0.751114 | -2.40088 | -2.51845 |

Table 18--Continued

|  |  |  | T* = 20 |  |  |
|---|---|---|---|---|---|
| n* | $C_1$ | $C_2$ | $C_3$ | $C_4$ | $C_5$ |
| 0.85 | 7.69714 | 21.9907 | -8.11816 | -56.3828 | -62.4961 |
| 0.65 | 1.37323 | 4.37946 | 3.75997 | -9.88257 | -17.105 |

Table 19

Values $b_2$ Versus $b_3$ to Give Correct P at T* = 6.11, 10 and 20

| T* | $b_2$ | $b_3$ |  |
|---|---|---|---|
| 6.11 |  | n* = 0.85 | n* = 0.65 |
|  | -0.20 | 0.140 | 0.196 |
|  | -0.15 | 0.118 | 0.164 |
|  | -0.10 | 0.097 | 0.099 |
|  | -0.05 | 0.076 | 0.067 |
|  | 0 | 0.055 | 0.035 |
|  | 0.05 | 0.034 | 0.003 |
|  | 0.10 | 0.014 | -0.029 |
|  | 0.15 | -0.006 | -0.061 |
|  | 0.20 | -0.025 | -0.093 |
| 10 | -0.20 | 0.135 | 0.188 |
|  | -0.15 | 0.115 | 0.16 |

| T* | b2 | b3 | |
|---|---|---|---|
| | | n* = 0.85 | n* = 0.65 |
| | -0.10 | 0.096 | 0.131 |
| | -0.05 | 0.077 | 0.103 |
| | 0 | 0.058 | 0.075 |
| | 0.05 | 0.401 | 0.047 |
| | 0.10 | 0.022 | 0.02 |
| | 0.15 | 0.005 | -0.008 |
| | 0.20 | -0.121 | -0.062 |
| 20 | -0.20 | 0.099 | 0.047 |
| | -0.15 | 0.088 | 0.053 |
| | -0.10 | 0.077 | 0.058 |
| | -0.05 | 0.065 | 0.060 |
| | 0 | 0.052 | 0.058 |
| | 0.05 | 0.037 | 0.046 |
| | 0.10 | 0.02 | 0.18 |
| | 0.15 | 0.072 | -0.33 |

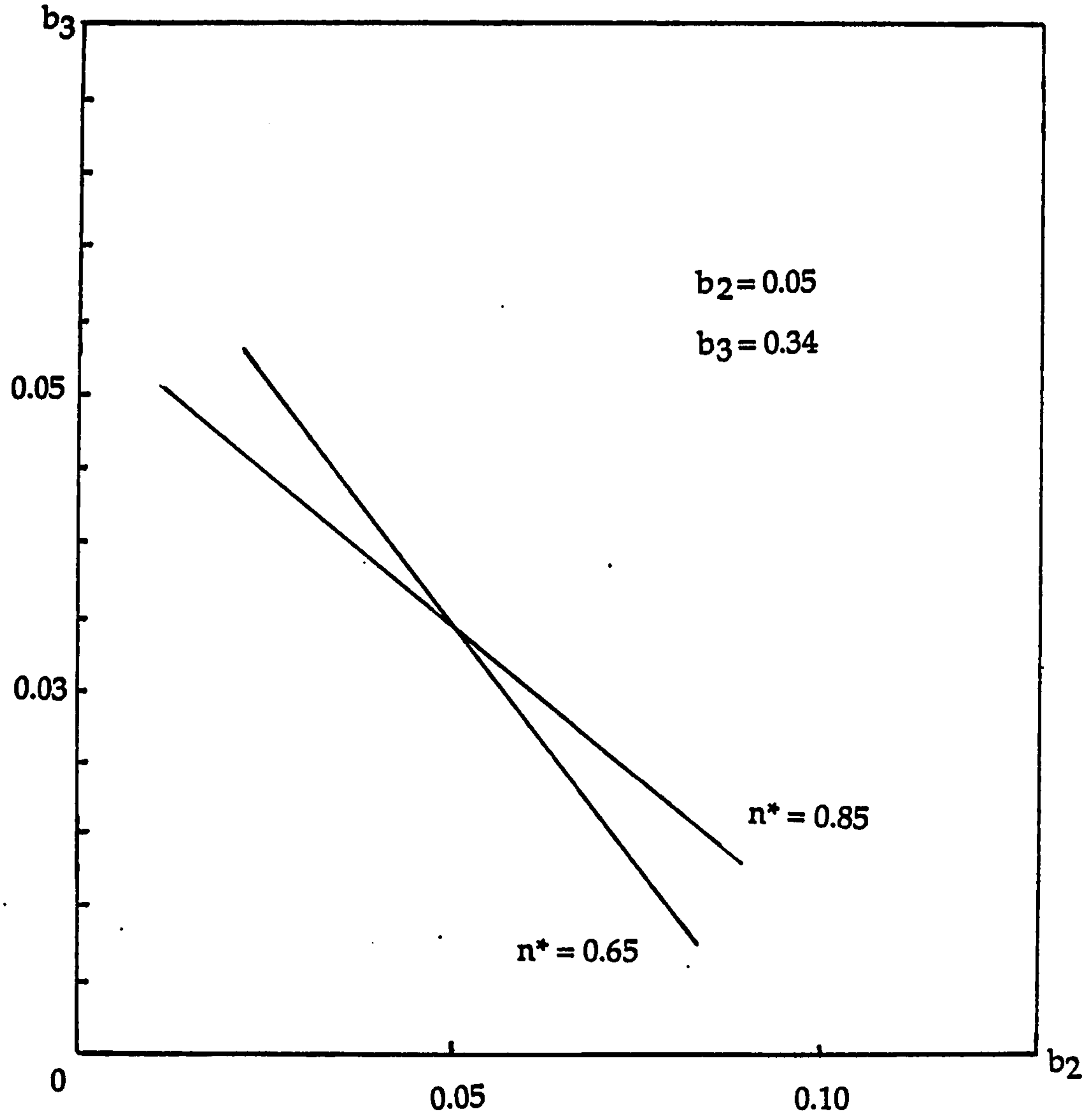

Figure 16. b2 Versus b3 of P* at T* = 6.11

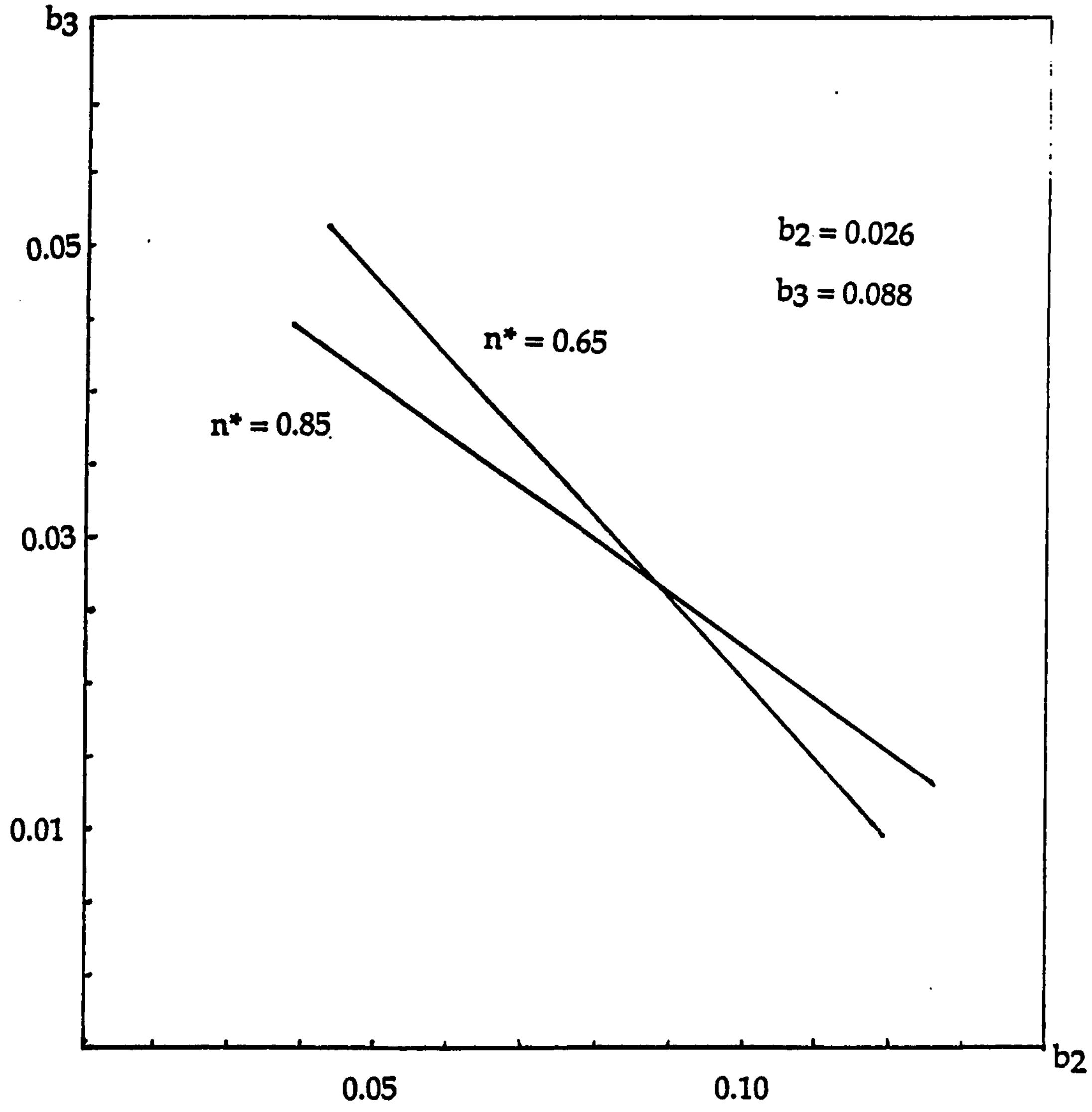

Figure 17. $b_2$ Versus $b_3$ of $P^*$ at $T^* = 10$

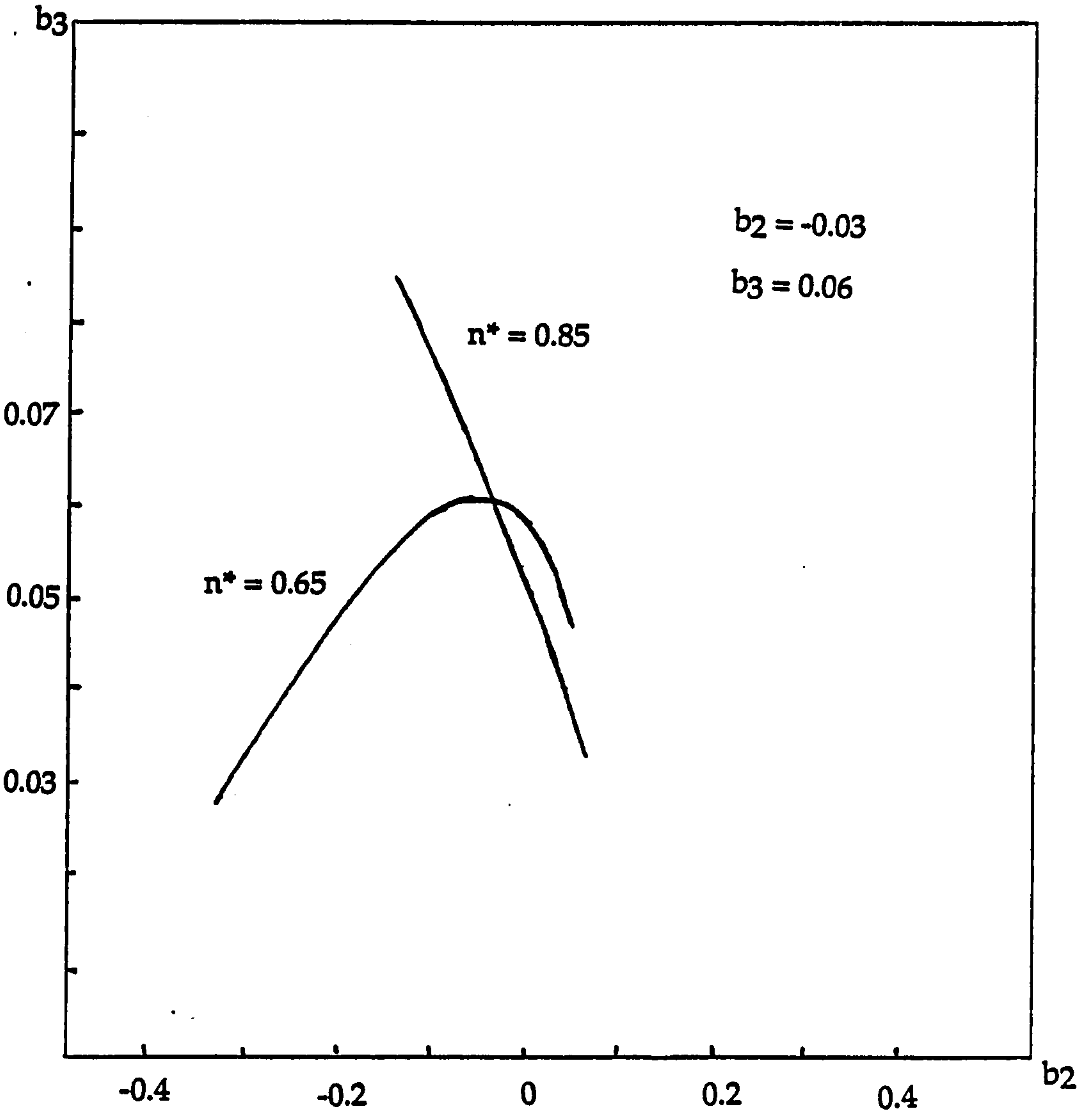

Figure 18. $b_2$ Versus $b_3$ of $P^*$ at $T^* = 20$

Table 20

P* and U* from Best Fit Parameter of Equation T at T* = 6.11, 10 and 20

| T* | n* | P* | U* |
|---|---|---|---|
| 6.11 | 0.001 | 1.001 | 0.999 |
| | 0.10 | 1.143 | 0.934 |
| | 0.30 | 1.632 | 0.789 |
| | 0.50 | 2.675 | 0.626 |
| | 0.70 | 4.942 | 0.461 |
| | 0.80 | 6.930 | 0.387 |
| 10 | 0.001 | 1.002 | 1.0 |
| | 0.10 | 1.181 | 0.962 |
| | 0.30 | 1.759 | 0.874 |
| | 0.50 | 2.902 | 0.774 |
| | 0.70 | 5.333 | 0.673 |
| | 0.80 | 7.503 | 0.628 |
| | 0.85 | 8.978 | 0.608 |
| 20 | 0.001 | 1.002 | 1 |
| | 0.10 | 1.210 | 0.982 |
| | 0.30 | 1.853 | 0.938 |
| | 0.45 | 2.659 | 0.901 |
| | 0.60 | 3.979 | 0.862 |
| | 0.75 | 6.262 | 0.825 |
| | 0.85 | 8.752 | 0.805 |

Table 20--Continued

| | | |
|---|---|---|
| $T^* = 6.11$ | $b_2 = 0.05$ | $b_3 = 0.34$ |
| $T^* = 10$ | $b_2 = 0.026$ | $b_3 = 0.088$ |
| $T^* = 20$ | $b_2 = -0.03$ | $b_3 = 0.06$ |

Table 21

Interpolated Values of P* and U* at T* = 6.11, 10 and 20

| T* | n* | P* | U* |
|---|---|---|---|
| 6.11 | 0.05 | 1.06 | 0.968 |
| | 0.10 | 1.143 | 0.934 |
| | 0.15 | 1.234 | 0.9 |
| | 0.20 | 1.343 | 0.864 |
| | 0.25 | 1.474 | 0.827 |
| | 0.30 | 1.631 | 0.789 |
| | 0.35 | 1.822 | 0.75 |
| | 0.40 | 2.454 | 0.709 |
| | 0.45 | 2.334 | 0.668 |
| | 0.50 | 2.675 | 0.626 |
| | 0.55 | 3.089 | 0.584 |
| | 0.60 | 3.592 | 0.541 |
| | 0.65 | 4.203 | 0.500 |
| | 0.70 | 4.942 | 0.460 |

Table 21--Continued

| T* | n* | P* | U* |
|---|---|---|---|
| 6.11 | 0.75 | 5.840 | 0.423 |
| | 0.80 | 6.932 | 0.387 |
| | 0.85 | 8.265 | 0.355 |
| | 0.90 | 9.908 | 0.367 |
| | 0.95 | 11.964 | 0.302 |
| | 1.00 | 14.595 | 0.281 |
| 10 | 0.05 | 1.084 | 0.981 |
| | 0.10 | 1.181 | 0.962 |
| | 0.15 | 1.294 | 0.941 |
| | 0.20 | 1.424 | 0.92 |
| | 0.25 | 1.578 | 0.898 |
| | 0.30 | 1.759 | 0.874 |
| | 0.35 | 1.973 | 0.85 |
| | 0.40 | 2.228 | 0.825 |
| | 0.45 | 2.533 | 0.8 |
| | 0.50 | 2.999 | 0.774 |
| | 0.55 | 3.342 | 0.748 |
| | 0.60 | 4.528 | 0.722 |
| | 0.65 | 4.528 | 0.697 |
| | 0.70 | 5.321 | 0.672 |
| | 0.75 | 6.290 | 0.649 |

Table 21--Continued.

| T* | n* | P* | U* |
|---|---|---|---|
| | 0.80 | 7.478 | 0.627 |
| | 0.85 | 8.94 | 0.608 |
| | 0.90 | 10.75 | 0.590 |
| | 0.95 | 13.02 | 0.576 |
| 20 | 0.05 | 1.098 | 0.991 |
| | 0.10 | 1.201 | 0.981 |
| | 0.15 | 1.337 | 0.971 |
| | 0.20 | 1.483 | 0.961 |
| | 0.25 | 1.652 | 0.949 |
| | 0.30 | 1.847 | 0.937 |
| | 0.35 | 2.072 | 0.925 |
| | 0.40 | 2.335 | 0.912 |
| | 0.45 | 2.643 | - |
| | 0.50 | 3.005 | 0.75 |
| | 0.55 | 3.432 | 0.872 |
| | 0.60 | 3.941 | 0.849 |
| | 0.65 | 4.548 | 0.837 |
| | 0.70 | 5.279 | 0.825 |
| | 0.75 | 6.164 | 0.814 |
| | 0.80 | 7.242 | 0.804 |
| | 0.85 | 8.561 | 0.795 |
| | 0.90 | 10.18 | 0.798 |

Table 21--Continued

Pade' Coefficients of P*

| Coefficients | T* = 6.11 | T* = 10 | T* = 20 |
|---|---|---|---|
| $a_1$ | -0.796005 | -0.543945 | 1.10059 |
| $a_2$ | 1.07625 | 0.468262 | 0.627197 |
| $a_3$ | 0.312088 | 0.123291 | 0.069141 |
| $a_4$ | -2.00598 | -2.11353 | -0.727051 |
| $a_5$ | 1.63034 | 1.64893 | -0.4375 |
| $a_6$ | -0.515259 | -0.469604 | 0.357178 |

Pade' Coefficients of U*

| Coefficients | T* = 6.11 | T* = 10 | T* = 20 |
|---|---|---|---|
| $a_1$ | -1.55066 | -1.00244 | -3.40989 |
| $a_2$ | 0.79483 | 0.33887 | 3.17958 |
| $a_3$ | -0.0532837 | 0.203613 | -1.20073 |
| $a_4$ | -0.911346 | -0.635254 | -3.235 |
| $a_5$ | 0.380432 | 0.157715 | 2.71347 |
| $a_6$ | 0.210236 | 0.249512 | -1.02891 |

Figures 21, 22, 23, 24, 25 and 26 show results of P* versus n* at T* = 6.11, 10 and 20. As noted, P* differs slightly fron "exact" results anly at high densities. Graphs are drawn to show radial distribution function as the function of distance x at three temperatures, T* = 6.11, 3.3333 and 1.8 for density n* = 0.75.

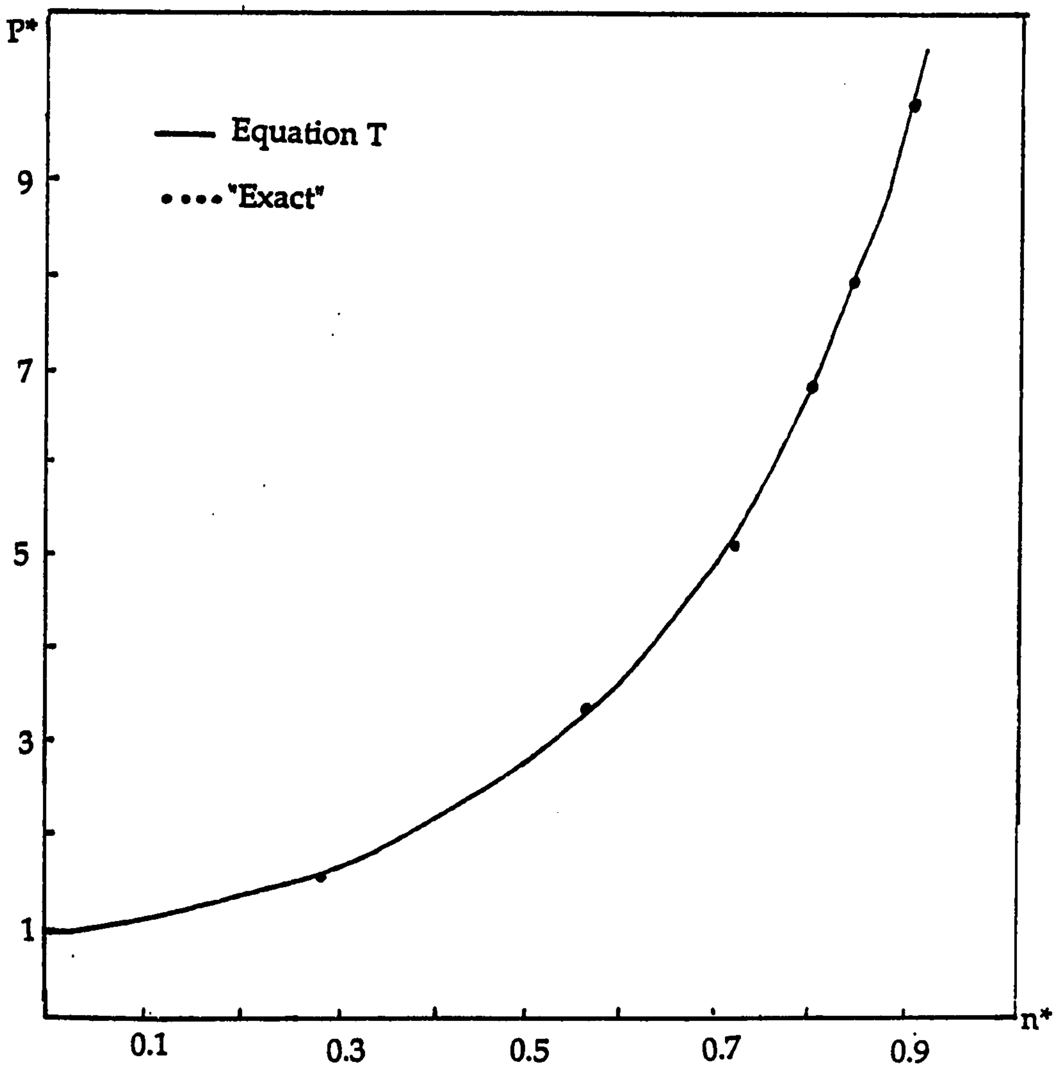

Figure 19. P* Versus n* at T* = 6.11

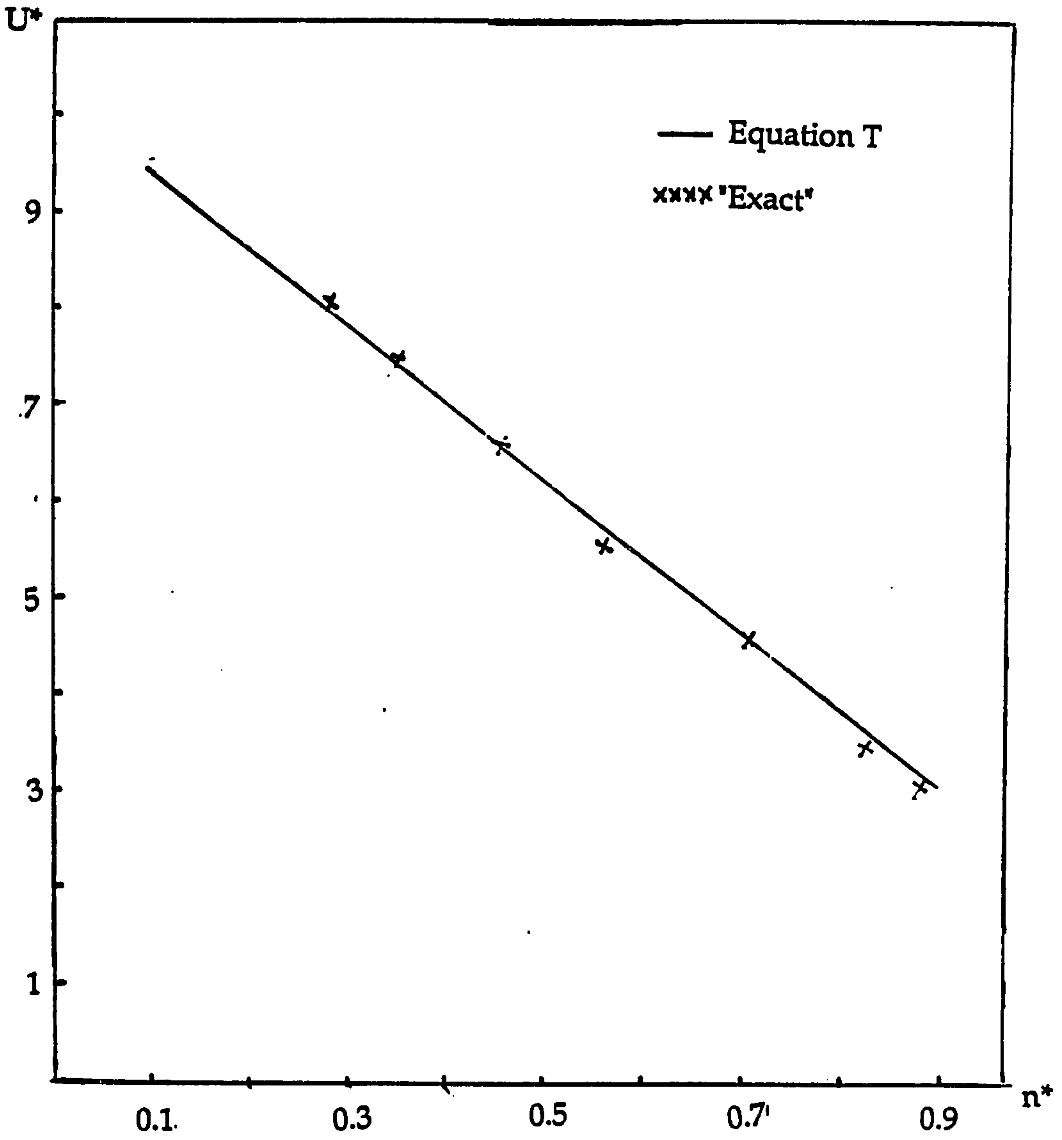

Figure 20. U* Versus n* at T* = 6.11

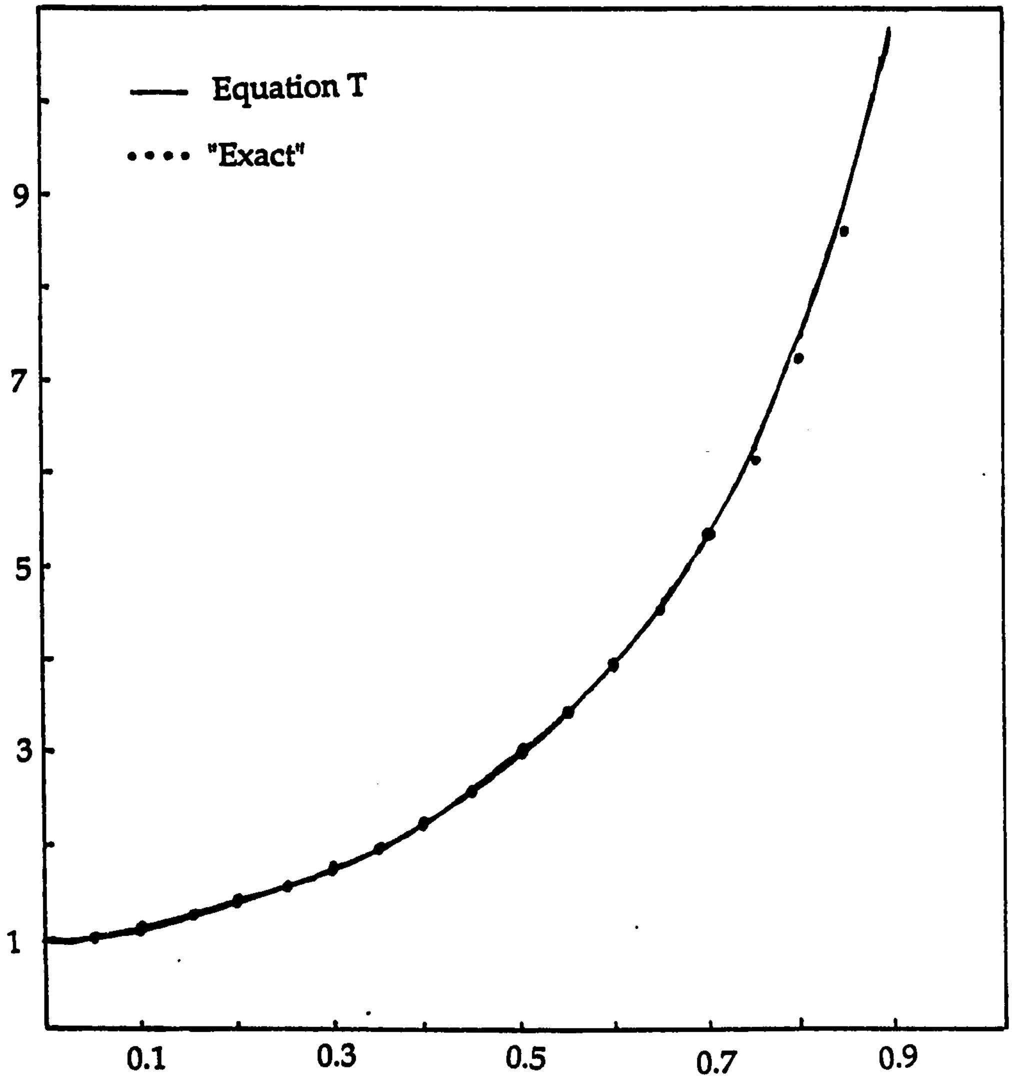

Figure 21. P*'Versus n* at T* = 10

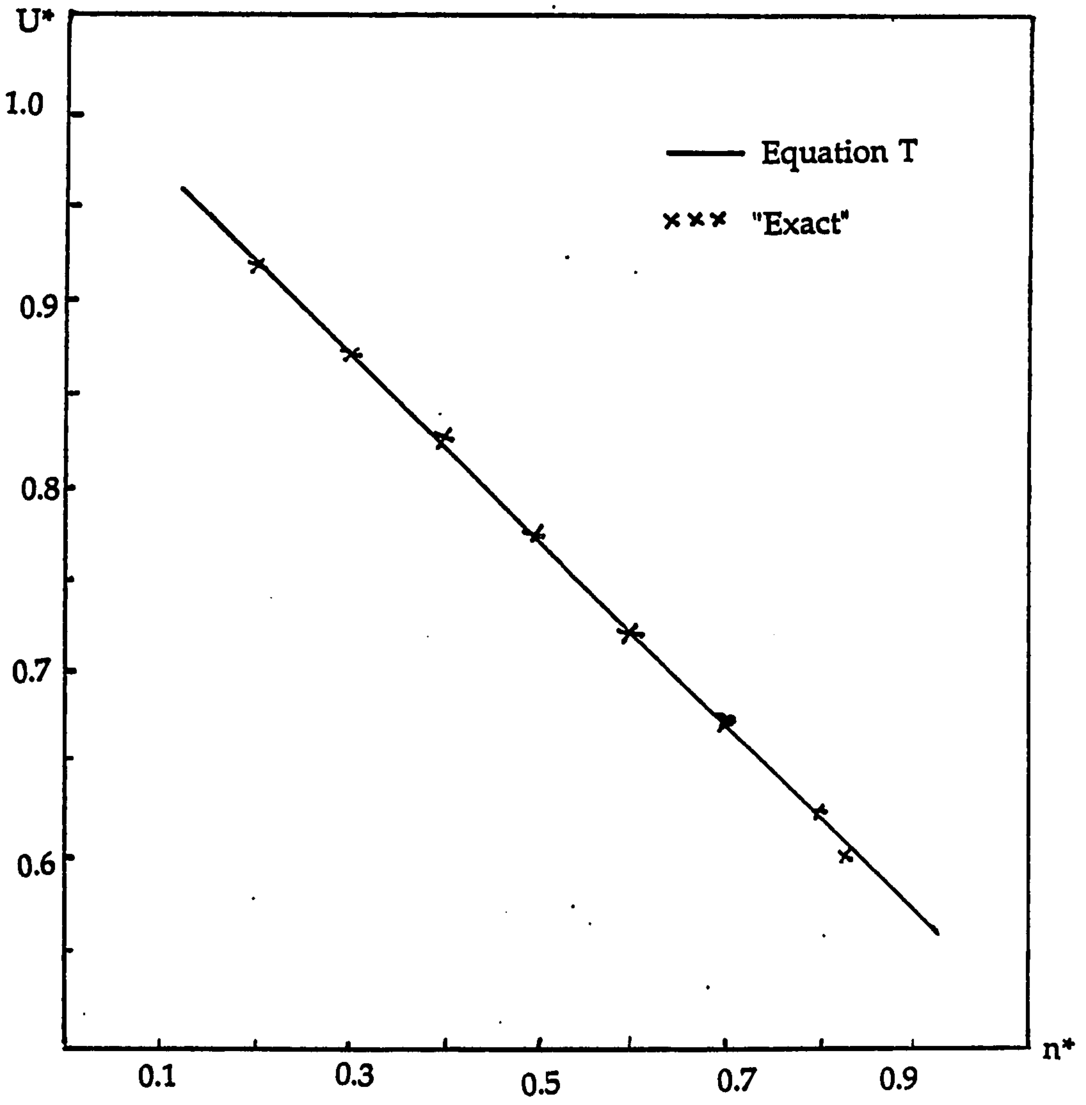

Figure 22. U* Versus n* at T* = 10

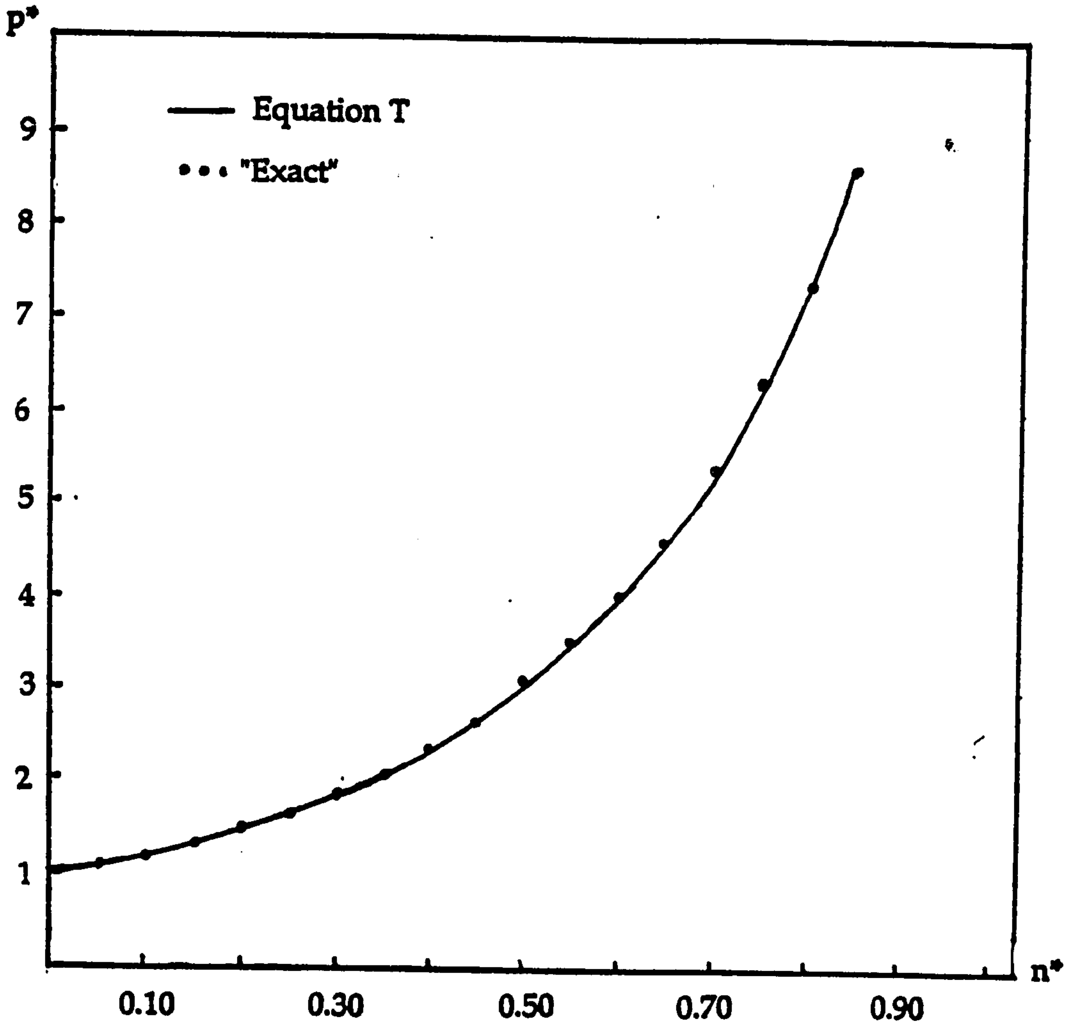

Figure 23 P* Versus n* at T* = 20

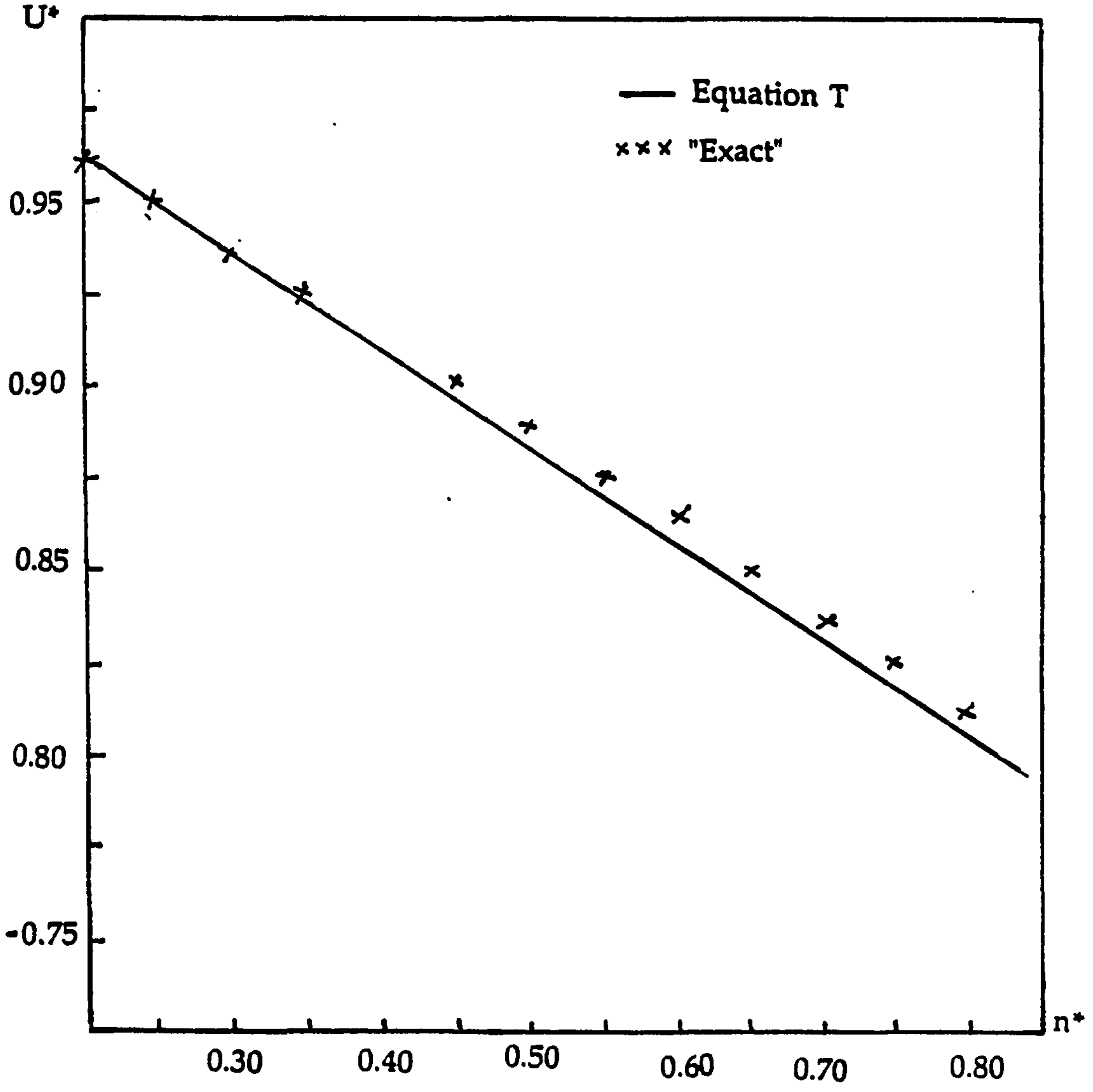

Figure 24 U* Versus n* at T* = 20

Table 22

Radial Distribution Function at T* = 3.3333, 6.11 and 1.8

| x | g(x) | | |
|---|---|---|---|
| | T* = 6.11 | T* = 10 | T* = 20 |
| 0.0179 | 0 | 0 | 0 |
| 0.1250 | 0 | 0 | 0 |
| 0.2500 | 0 | 0 | 0 |
| 0.3750 | 0 | 0 | 0 |
| 0.5000 | 0 | 0 | 0 |
| 0.6250 | 0 | 0 | 0 |
| 0.7500 | 0 | 0 | 0 |
| 0.8750 | 0 | 0 | 0 |
| 1.0000 | 3.495 | 2.748 | 3.378 |
| 1.0714 | 2.554 | 2.389 | 2.478 |
| 1.1250 | 2.051 | 2.245 | 2.064 |
| 1.1964 | 1.565 | 1.890 | 1.644 |
| 1.2500 | 1.304 | 1.550 | 1.385 |
| 1.3214 | 1.062 | 1.234 | 1.112 |
| 1.3750 | 0.944 | 0.941 | 0.971 |
| 1.4464 | 0.853 | 0.825 | 0.865 |
| 1.5000 | 0.824 | 0.840 | 0.842 |
| 1.5714 | 0.703 | 0.548 | 0.644 |
| 1.6250 | 0.725 | 0.651 | 0.682 |

Table 22--Continued

| x | g(x) | | |
|---|---|---|---|
| | $T^* = 6.11$ | $T^* = 3.3333$ | $T^* = 1.4$ |
| 1.6964 | 0.775 | 0.7360 | 0.754 |
| 1.7500 | 0.825 | 0.822 | 0.817 |
| 1.8214 | 0.902 | 0.929 | 0.707 |
| 1.8750 | 0.968 | 1.002 | 0.977 |
| 1.9464 | 1.063 | 1.089 | 1.072 |
| 2.0000 | 1.139 | 1.145 | 1.142 |
| 2.0714 | 1.186 | 1.186 | 1.187 |
| 2.1250 | 1.171 | 1.189 | 1.178 |
| 2.1964 | 1.120 | 1.162 | 1.136 |
| 2.2500 | 1.074 | 1.123 | 1.092 |
| 2.3214 | 1.016 | 1.052 | 1.03 |
| 2.3750 | 0.980 | 0.994 | 0.987 |
| 2.4464 | 0.945 | 0.927 | 0.941 |
| 2.5000 | 0.928 | 0.889 | 0.916 |
| 2.5714 | 0.921 | 0.870 | 0.904 |
| 2.6250 | 0.927 | 0.883 | 0.912 |
| 2.6964 | 0.946 | 0.922 | 0.936 |
| 2.7500 | 0.965 | 0.957 | 0.96 |
| 2.8214 | 0.992 | 1.000 | 0.992 |
| 2.8750 | 1.011 | 1.026 | 1.014 |
| 2.9464 | 1.031 | 1.049 | 1.036 |
| 3.0000 | 1.041 | 1.058 | 1.046 |

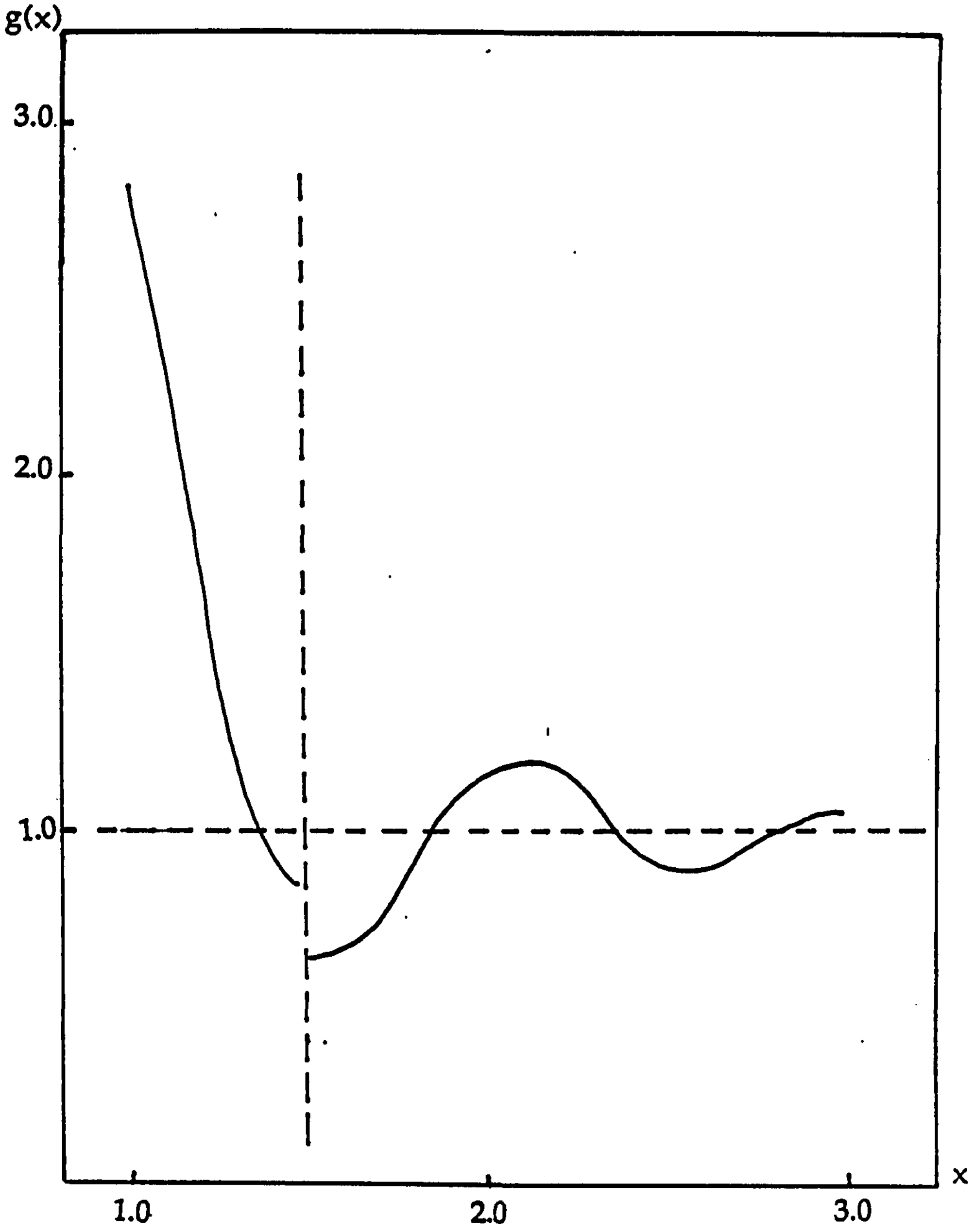

Figure 25. Radial Distribution Function at T* = 1.8 (n* = 0.75)

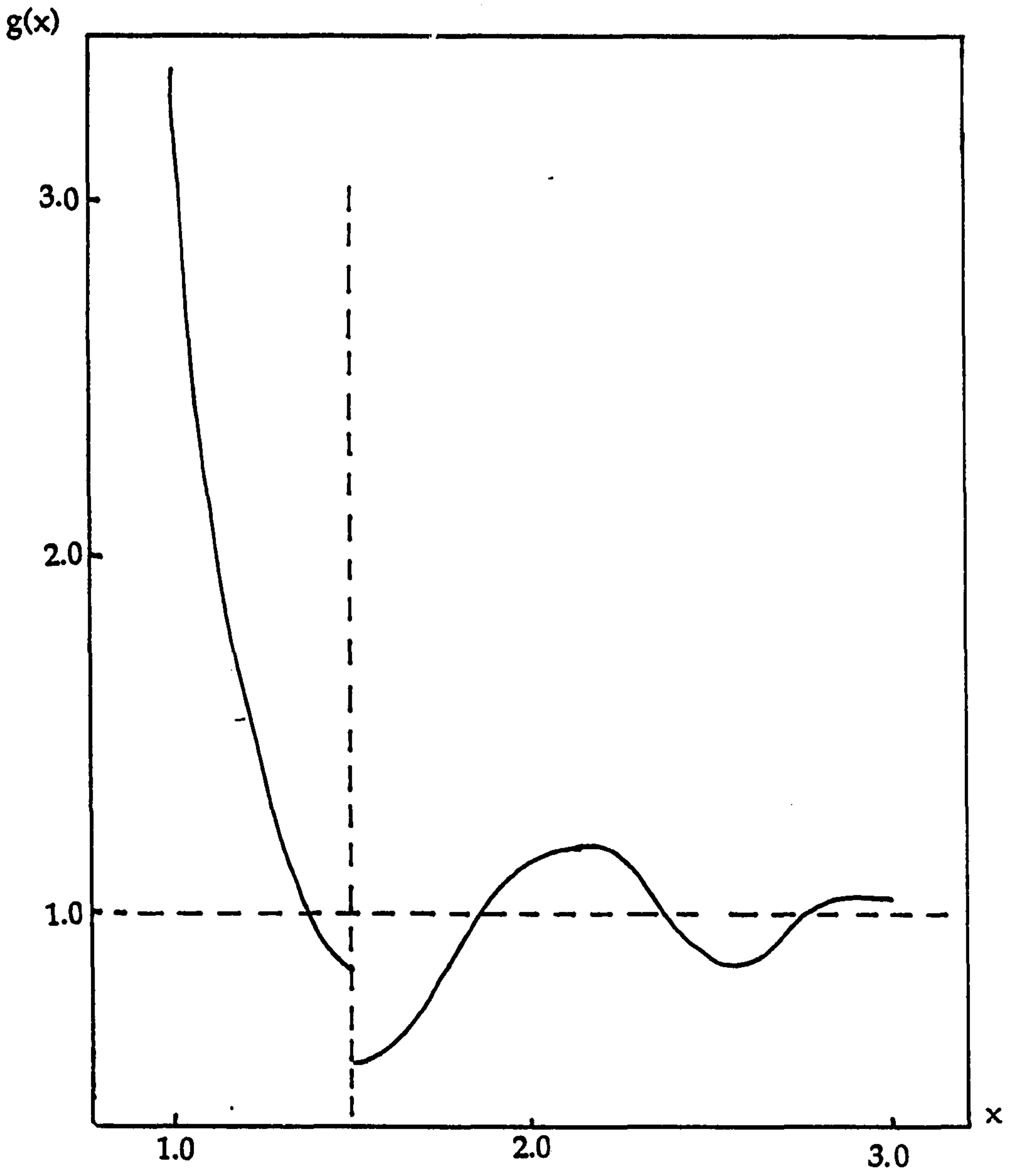

Figure 26. Radial Distribution Function at T* = 3.3333 (n* = 0.75)

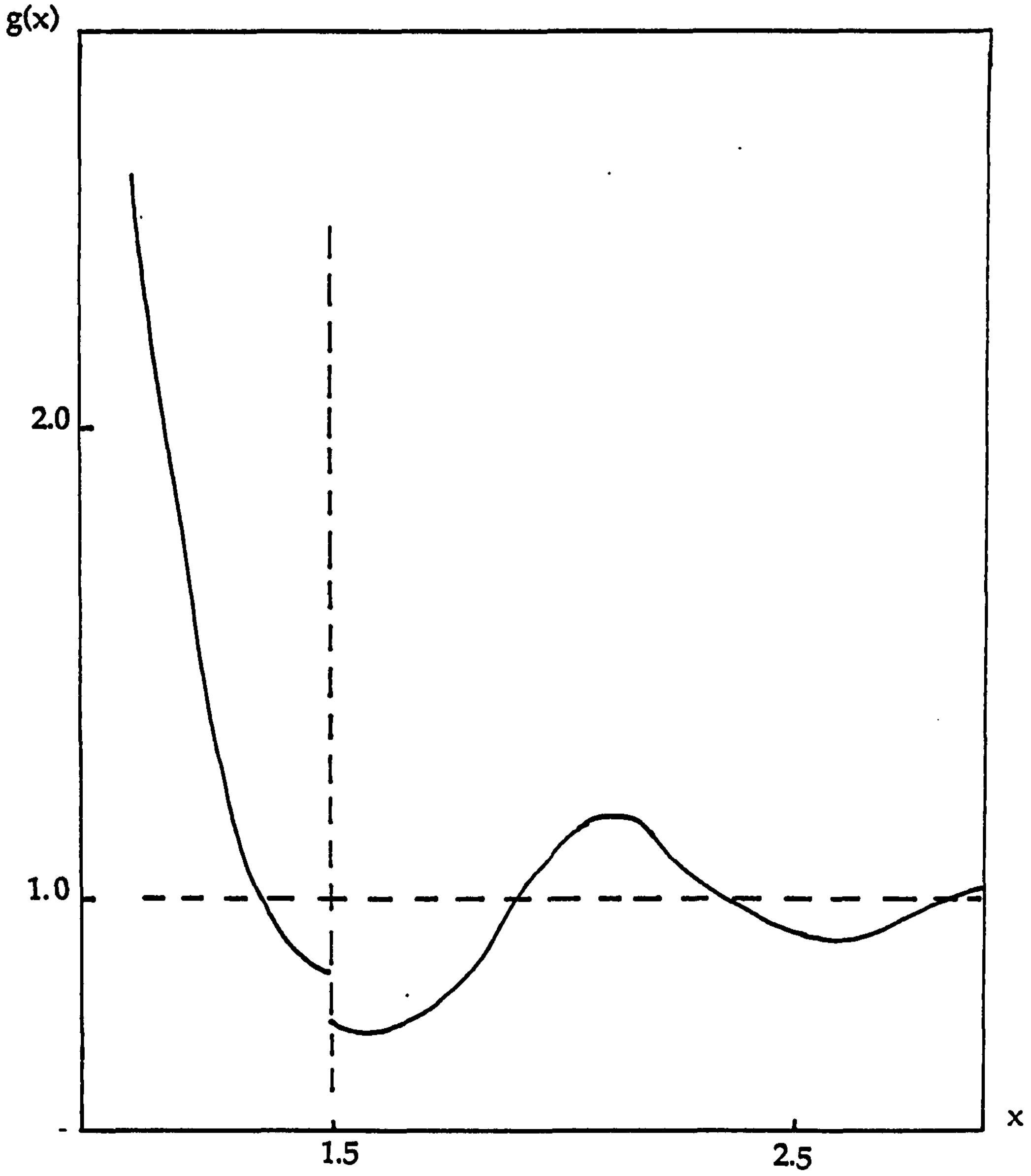

Figure 27. Radial Distribution Function at $T^* = 6.11$ ($n^* = 0.75$)

# CHAPTER V

## SUMMARY AND CONCLUSIONS

A two parametric integral equation, equation T, was studied where square-well potential ia an assumed potential used for the system studied. Radial distribution functions were computed from high temperature, $T^*=$ 20, to low temperature $T^* = 1.4$, in the gas region. Comparisons were made with the "exact" Monte Carlo results that were read from Alder's graphs, equation C and results from Carley's combinaticn of pertübation and integral equation method. Theoretical results were used for comparisons to avoid the task of determining the interpartical forces. Thus, it is certain that if the results obtained differ from the attempted results, it is because of theoretical and numerical approximation involved in using the integral equation.

Equation T was initially solved for two densities $n^* = 0.85$ and $n^* = 0.65$ at seven selected temperatures where values of $b_2$ and $b_3$ were chosen to give close agreements to established "exact" results. Good agreements were found for temperatures $T^* = 6.11, 3.3333$ and $6.11$ at low and as well as high densities. At temperature $T^* = 10$ amd $T^* = 20$ a small deviation from "exact" (equation C) occurred at high densities which shows that $b_3$ becomes reasonably important and gives significant effect at high densities and on the results obtained. This is because $b_3$ appears only in higher densities terms in the density expansion.

becomes reasonably important and gives significant effect at high densities and, thus,

At $T^* = 1.8$, deviations occurred at low and at high densities except at densities $n^* = 0.85$ and $n^* = 0.65$. These are expected since the parameters of equation T, used to find coefficients for the least square fit equation, were chosen to give agreements to the "exact" values. Best fit parameters were obtained at much lower temperature ($T^* = 1.4$), but no agreement with the "exact" values was found because no convergence could be obtained at all densities. If there were convergences, they usually gave questionable results. No comparisons can be made and therefore, this concludes that equation T does not work well in low temperature gas region.

This study shows that equation T works well at low temperatures and it is better than equation C. But equation T is not convenient to work with since it deals with two parameters which require a lot more work. When comparing results from equation T using square-well potential with results using Lennard Jones potential, it is shown that Equation T using Lennard Jones potential does gives better results.

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# APPENDIX A

## EQUATION T RESULTS

This appendix lists all results of numerical solution of solving integral equation T using the main program. The following notations are used.

| Notations | Discriptions |
|---|---|
| $b_2$ and $b_3$ | Values of parameters in equation T |
| $n^*$ | Reduced number density. |
| $T^*$ | Reduced temperature. |
| N | A indicates 75 points were used to specify the function with intervals of 0.07142857.<br>B indicates 297 points were used to specify the function with an interval of 0.01785714. |
| SDSS | Measure of the difference between the final guessed value of S and computed value of S. This is also to indicate how good the convergence is. The smaller the value of SDSS, the better is the convergence. |
| $P^*$ and $U^*$ | Reduced pressure and energy, calculated from the radial distribution function. |

Table 23

Complete Results of P* and U* of Equation T

| b2 | b3 | n* | T* | N | SDSS | P* | U* |
|---|---|---|---|---|---|---|---|
| 0 | 0 | 0.85 | 3.3333 | A | .195E-5 | 6.7563782 | -0.19625568 |
| | | | | B | .977E-5 | 7.1476440 | -0.19142985 |
| 0 | 0.1667 | | | A | .166E-5 | 7.7022090 | -0.18968117 |
| | | | | B | .745E-6 | 8.5003777 | -0.18472409 |
| 0.5 | 0 | | | A | .168E-5 | 8.80351477 | -0.19194698 |
| | | | | B | .214E-5 | 8.81336816 | -0.18879616 |
| 0.1175 | 0.0092 | | | A | .448E-5 | 7.21554848 | -0.19323182 |
| | | | | B | .178E-5 | 7.745555 | -0.18866730 |
| 0.4 | 0.05 | | | A | .704E-6 | 8.0046206 | -0.19041419 |
| | | | | B | .746E-6 | 8.7976208 | -0.18666637 |
| 0.5 | 0.1667 | | | A | .547E-6 | 8.4585466 | -0.18850577 |
| | | | | B | .701E-5 | 9.4561443 | -0.18488586 |
| 0.3 | 0.3 | | | A | .533E-6 | 8.4819536 | -0.18567610 |
| | | | | B | .862E-5 | 9.5448084 | -0.181123889 |
| 0 | 0 | 0.65 | | A | .215E-7 | 3.4735594 | 0.070326626 |
| | | | | B | .246E-6 | 3.5785537 | 0.070133805 |
| 0 | 0.1667 | | | A | .311E-6 | 3.6506388 | 0.07188600 |
| | | | | B | .312E-6 | 3.7948359 | 0.071707368 |
| 0.5 | 0 | | | A | .294E-6 | 3.8827496 | 0.075995028 |
| | | | | B | .310E-6 | 4.0504513 | 0.075964332 |

Table 23--Continued

| $b_2$ | $b_3$ | $n^*$ | $T^*$ | N | SDSS | $P^*$ | $U^*$ |
|---|---|---|---|---|---|---|---|
| 0.1175 | 0.0092 | 0.65 | 3.3333 | A | .489E-6 | 3.5983171 | 0.072121382 |
| | | | | B | .144E-6 | 3.7221196 | 0.071987510 |
| 0.4 | 0.05 | | | A | .334E-6 | 3.8512378 | 0.075376868 |
| | | | | B | .342E-6 | 4.0166163 | 0.075325966 |
| 0.5 | 0.1667 | | | A | .290E-6 | 3.9894714 | 0.076633453 |
| | | | | B | .409E-6 | 4.1841631 | 0.076594055 |
| 0.3 | 0.3 | | | A | .232E-6 | 3.9553180 | 0.075655818 |
| | | | | B | .812E-6 | 4.1519780 | 0.075578034 |
| 0 | 0 | 0.85 | 2.6 | A | .319E-5 | 6.4947963 | -0.53877711 |
| | | | | B | .301E-5 | 6.9079013 | -0.53156531 |
| -0.7 | 0.6 | | | A | .179E-5 | 7.7382021 | -0.52575164 |
| | | | | B | .186E-2 | 8.9931068 | -0.51687109 |
| -0.8 | 0.65 | | | A | .154E-5 | 7.8077855 | -0.5268656 |
| | | | | B | .514E-2 | 9.0776358 | -0.52129400 |
| -0.85 | 0.40 | | | A | .733E-6 | 7.1648660 | -0.54195571 |
| | | | | B | .242E-5 | 8.5320864 | -0.53257334 |
| -0.7 | 0.4 | | | A | .610E-5 | 7.1859102 | -0.53537834 |
| | | | | B | .195E-5 | 8.3575621 | -0.5624869 |
| -0.85 | 0.6 | | | A | .159E-5 | 7.6902852 | -0.52977979 |
| | | | | B | .302E-3 | 9.1306143 | -0.52034461 |
| -0.8 | 0.45 | | | A | .178E-5 | 7.3256750 | -0.53416805 |
| | | | | B | .188E-5 | 8.6196613 | -0.5653563 |

Table 23--Continued

| $b_2$ | $b_3$ | $n^*$ | $T^*$ | N | SDSS | $P^*$ | $U^*$ |
|---|---|---|---|---|---|---|---|
| 0 | 0 | 0.65 | 2.6 | A | .117E-6 | 3.1803179 | -0.20225751 |
| | | | | B | .321E-6 | 3.2923281 | -0.20172048 |
| -0.7 | 0.6 | | | A | .325E-6 | 3.2923281 | -0.20668876 |
| | | | | B | .300E-6 | 3.2931020 | -0.20647514 |
| -0.8 | 0.65 | | | A | .306E-6 | 3.1024172 | -0.20795941 |
| | | | | B | .525E-6 | 3.2643993 | -0.20783186 |
| -0.85 | 0.40 | | | A | .358E-6 | 2.7301290 | -0.21499109 |
| | | | | B | .530E-6 | 2.8277113 | -0.21530366 |
| -0.8 | 0.45 | | | A | .383E-6 | 2.872043 | -0.21179390 |
| | | | | B | .709E-6 | 2.9888151 | -0.21187568 |
| -0.70 | 0.40 | | | A | .379E-6 | 2.9180334 | -0.21002758 |
| | | | | B | .304E-6 | 3.0313866 | -0.20997322 |
| -0.85 | 0.60 | | | A. | .235E-6 | 2.9984286 | -0.21021509 |
| | | | | B | .795E-6 | 3.1471994 | -0.21022594 |
| 0 | 0 | 0.85 | 1.8 | A | .722E-6 | 5.9623165 | -1.2378807 |
| | | | | B | .345E-5 | 6.4180951 | -1.2245107 |
| 0.1175 | 0.0092 | | | A | .124E-5 | 6.2815056 | -1.2406933 |
| | | | | B | .148E-5 | 6.8633385 | -1.2278628 |
| -0.225 | 0.15 | | | A | .369E-6 | 6.0035253 | -1.2277236 |
| | | | | B | .170E-5 | 6.5870590 | -1.2131097 |
| -0.15 | 0.10 | | | A | .348E-5 | 5.9852977 | -1.2306306 |
| | | | | B | .151E-5 | 6.5224748 | -1.2163684 |

Table 23--Continued

| $b_2$ | $b_3$ | n* | T* | N | SDSS | P* | U* |
|---|---|---|---|---|---|---|---|
| -0.4 | 0.20 | | | A | .281E-5 | 6.373818 | -1.2247856 |
| | | | | B | .144E-5 | 6.373818 | -1.2097538 |
| -0.3 | 0.1 | 0.85 | 1.8 | A | .522E-5 | 5.5622587 | -1.2304845 |
| | | | | B | .368E-4 | 5.218432 | -1.2307656 |
| -0.6 | 0.2 | | | A | .164E-4 | 5.218432 | -1.2307656 |
| | | | | B | .392E-5 | 5.7503672 | -1.2247488 |
| 0 | 0 | 0.65 | | A | .207E-6 | 2.6026130 | -0.76647329 |
| | | | | B | .895E-6 | 2.728990 | -0.76331866 |
| 0.1175 | 0.0092 | | | A | .825E-6 | 2.6542280 | -0.76720524 |
| | | | | B | .756E-6 | 2.7956033 | -0.76410472 |
| -0.225 | 0.15 | | | A | .195E-6 | 2.5629094 | -0.76446271 |
| | | | | B | .319E-6 | 2.6804533 | -0.76120317 |
| -0.15 | 0.1 | | | A | .325E-6 | 2.577236 | -0.76502335 |
| | | | | B | .295E-6 | 2.6976142 | -0.76178718 |
| -0.4 | 0.2 | | | A | .377E-6 | 2.4938669 | -0.76407599 |
| | | | | B | .383E-6 | 2.5966499 | -0.76080859 |
| -0.3 | 0.1 | | | A | .270E-6 | 2.5009351 | -0.76482940 |
| | | | | B | .367E-6 | 2.6030908 | -0.76158023 |
| -0.6 | 0.2 | | | A | .481E-6 | 2.3678517 | -0.76165688 |
| | | | | B | .346E-6 | 2.44445951 | -0.76165688 |
| 0 | 0 | 0.85 | 1.4 | A | .499E-6 | 5.4541912 | -1.8960524 |
| | | | | B | .274E-6 | 5.9487991 | -1.8753595 |

Table 23--Continued

| $b_2$ | $b_3$ | n* | T* | N | SDSS | P* | U* |
|---|---|---|---|---|---|---|---|
| 0.1175 | 0.0092 | | | A | .180E-5 | 5.7010589 | -1.9056975 |
| | | | | B | .242E-5 | 6.3155351 | -1.8850944 |
| 0.05 | -0.2 | | | A | .970E-5 | 4.9422574 | -1.9179475 |
| | | | | B | .282E-5 | 5.1114421 | -1.8995726 |
| 0.15 | -0.1 | | | A | .556E-5 | 5.5323400 | -1.9186985 |
| | | | | B | .105E-5 | 6.0233474 | -1.9002521 |
| 0.15 | -0.2 | | | A | .436E-5 | 5.2487855 | -1.9311764 |
| | | | | B | .294E-5 | 5.5570016 | -1.9146433 |
| 0.2 | -0.1 | | | A | .240E-5 | 5.6390958 | -1.9253347 |
| | | | | B | .280E-5 | 6.1852498 | -1.9076796 |
| 0.2 | -0.2 | | | A | .310E-5 | 5.3838220 | -1.9399796 |
| | | | | B | .313E-5 | 5.7585845 | -1.9249921 |
| 0 | 0 | 0.65 | | A | .403E-8 | 2.0803168 | -1.3063579 |
| | | | | B | .181E-6 | 2.2198944 | -1.2992847 |
| 0.1175 | 0.0092 | | | A | .226E-6 | 2.0894551 | -1.3105977 |
| | | | | B | .258E-6 | 2.2419636 | -1.3036809 |
| 0.05 | -0.2 | | | A | .102E-6 | 2.0330129 | -1.3059127 |
| | | | | B | .351E-6 | 2.1660993 | -1.3173382 |
| 0.15 | -0.1 | | | A | .221E-6 | 2.0620608 | -1.3146353 |
| | | | | B | .267E-6 | 2.2119348 | -1.3079607 |
| 0.15 | -0.1 | | | A | .241E-6 | 2.0344996 | -1.3173382 |
| | | | | B | .238E-6 | 2.1785436 | -1.3108687 |

Table 23--Continued

| $b_2$ | $b_3$ | n* | Γ* | N | SDSS | P* | U* |
|---|---|---|---|---|---|---|---|
| 0.2 | -0.1 | 0.65 | 1.4 | A | .208E-6 | 2.0616720 | -1.317056 |
| | | | | B | .354E-6 | 2.2171683 | -1.3164997 |
| 0.2 | -0.2 | | | A | .262E-6 | 2.0330451 | -1.3200130 |
| | | | | B | .376E-6 | 2.1827538 | -2.3136911 |
| 0 | 0 | 0.85 | 6.11 | A | .139E-5 | 7.1792774 | 0.35088563 |
| | | | | B | .591E-5 | 7.5357866 | 0.35281187 |
| 0.1175 | 0.0092 | | | A | .370E-5 | 7.7236438 | 0.35409856 |
| | | | | B | .172E-5 | 8.2241611 | 0.35589963 |
| 0.5 | 0.1667 | | | A | .834E-6 | 9.0869360 | 0.35988933 |
| | | | | B | .943E-6 | 10.037261 | 0.36122400 |
| 0.2 | 0.4 | | | A | .157E-6 | 9.2933311 | 0.36073309 |
| | | | | B | .1E-6 | 10.419754 | 0.36246794 |
| -0.25 | 0.3 | | | A | .182E-5 | 8.6014271 | 0.35578293 |
| | | | | B | .124E-5 | 9.6145306 | 0.35789371 |
| -0.1 | 0.5 | | | A | .665E-6 | 9.2697563 | 0.36001801 |
| | | | | B | .199E-5 | 10.479503 | 0.36201465 |
| 0.4 | - 0.1 | | | A | .109E-5 | 7.8236451 | 0.35543633 |
| | | | | B | .1E-5 | 8.2413292 | 0.35684812 |
| 0 | 0 | 0.65 | | A | .349E-6 | 3.9580369 | 0.50002831 |
| | | | | B | .308E-6 | 4.0520568 | 0.49940103 |
| 0.1175 | 0.0092 | | | A | .379E-6 | 4.1218262 | 0.50163329 |
| | | | | B | .371E-6 | 4.2368970 | 0.50106937 |

Table 23--Continued

| $b_2$ | $b_3$ | $n^*$ | $T^*$ | N | SDSS | $P^*$ | $U^*$ |
|---|---|---|---|---|---|---|---|
| 0.2 | 0.4 | 0.65 | 6.11 | A | .382E-6 | 4.6113076 | 0.50458729 |
| | | | | B | .421E-6 | 4.8197188 | 0.50405461 |
| -0.25 | 0.3 | | | A | .325E-6 | 4.1885924 | 0.50023568 |
| | | | | B | .514E-6 | 4.3494925 | 0.49951857 |
| -0.1 | 0.5 | | | A | .447E-6 | 4.52-5216 | 0.50302547 |
| | | | | B | .415E-6 | 4.8311807 | 0.50240046 |
| 0.4 | -0.1 | | | A | .330E-5 | 4.26 54905 | 0.50365484 |
| | | | | B | .412E-6 | 4.3882117 | 0.50320268 |
| 0.5 | 0.1667 | | | A | .297E-6 | 4.6078858 | 0.50557733 |
| | | | | B | .2E-6 | 4.7973838 | 0.50513256 |
| 0 | 0 | 0.85 | 10 | A | .543E-6 | 7.3795228 | 0.60439271 |
| | | | | B | .189E-5 | 7.7191029 | 0.60536534 |
| 0.1175 | 0.0092 | | | A | .109E-5 | 7.9648333 | 0.60683489 |
| | | | | B | .591E-5 | 8.4520158 | 0.60773838 |
| 0.2 | 0.4 | | | A | .219E-5 | 9.6292181 | 0.61150855 |
| | | | | B | .484E-5 | 10.746062 | 0.61232579 |
| -0.25 | 0.3 | | | A | .224E-5 | 8.9763136 | 0.60797733 |
| | | | | B | .465E-5 | 10.003480 | 0.60900182 |
| -0.1 | 0.5 | | | A | .648E-5 | 9.6360979 | 0.61086637 |
| | | | | B | .248E-5 | 10.845904 | 0.61181670 |
| 0.3 | 0.3 | | | A | .182E-5 | 9.4918928 | 0.61130762 |
| | | | | B | .182E-5 | 10.523094 | 0.61207241 |

Table 23--Continued

| $b_2$ | $b_3$ | $n^*$ | $T^*$ | N | SDSS | $P^*$ | $U^*$ |
|---|---|---|---|---|---|---|---|
| 0.5 | 0.1667 | 0.85 | 10 | A | .134E-5 | 9.3783969 | 0.61207241 |
|  |  |  |  | B | .341E-5 | 10.306882 | 0.61188203 |
| 0 | 0 | 0.65 |  | A | .388E-6 | 4.1898904 | 0.69659889 |
|  |  |  |  | B | .311E-6 | 4.2789631 | 0.6960755 |
| 0.1175 | 0.0092 |  |  | A | .369E-6 | 4.3713861 | 0.69774611 |
|  |  |  |  | B | .438E-6 | 4.4826107 | 0.69727618 |
| 0.3 | 0.3 |  |  | A | .281E-6 | 4.8907957 | 0.70009017 |
|  |  |  |  | B | .331E-6 | 5.0885949 | 0.69965845 |
| 0.2 | 0.4 |  |  | A | .282E-6 | 4.9211087 | 0.69997340 |
|  |  |  |  | B | .258E-6 | 5.1311197 | 0.69952011 |
| -0.25 | 0.3 |  |  | A | .538E-6 | 4.5001264 | 0.69711524 |
|  |  |  |  | B | .631E-6 | 4.6677880 | 0.69652909 |
| -0.1 | 0.5 |  |  | A | .262E-6 | 4.8464326 | 0.69902128 |
|  |  |  |  | B | .338E-6 | 5.0624571 | 0.69850061 |
| 0.5 | 0.1667 |  |  | A | .290E-6 | 4.8954854 | 0.70053422 |
|  |  |  |  | B | .411E-6 | 5.0824952 | 0.70014578 |
| 0 | 0 | 0.85 | 20 | A | .449E-5 | 7.5380487 | 0.80259097 |
|  |  |  |  | B | .247E-5 | 7.7190819 | 0.60536516 |
| 0.1175 | 0.0092 |  |  | A | .979E-6 | 8.1564054 | 0.80400765 |
|  |  |  |  | B | .131E-4 | 8.1564054 | 0.80400765 |
| 0.1 | 0.01 |  |  | A | .600E-5 | 8.1048183 | 0.80387586 |
|  |  |  |  | B | .535E-5 | 8.5718718 | 0.80425507 |
| 0.05 | 0.05 |  |  | A | .203E-5 | 8.321204 | 0.80403262 |

Table 23--Continued

| $b_2$ | $b_3$ | $n^*$ | $T^*$ | N | SDSS | $P^*$ | $U^*$ |
|---|---|---|---|---|---|---|---|
| 0.05 | 0.05 | 0.85 | 20 | B | .374E-5 | 8.8895731 | 0.80441469 |
| 0.1 | 0.04 | | | A | .270E-5 | 8.3739252 | 0.80426979 |
| | | | | B | .353E-5 | 8.9375582 | 0.80464178 |
| 0.15 | 0.05 | | | A | .936E-6 | 8.5706682 | 0.80468971 |
| | | | | B | .221E-5 | 9.1844282 | 0.80504686 |
| 0.01 | 0.1667 | | | A | .513E-6 | 8.9719877 | 0.80493087 |
| | | | | B | .128E-5 | 9.7900686 | 0.80530363 |
| 0 | 0 | 0.65 | | A | .194E-6 | 4.3746872 | 0.84912217 |
| | | | | B | .194E-6 | 4.4599791 | 0.84886167 |
| 0.1175 | 0.0092 | | | A | .198E-6 | 4.5697279 | 0.84976965 |
| | | | | B | .382E-6 | 4.6780186 | 0.84947747 |
| 0.1 | 0.01 | | | A | .556E-6 | 4.5488195 | 0.84969598 |
| | | | | B | .416E-6 | 4.6549182 | 0.84940028 |
| 0.05 | 0.05 | | | A | .416E-6 | 4.5732498 | 0.84966612 |
| | | | | B | .323E-6 | 4.6879373 | 0.84938237 |
| 0.1 | 0.04 | | | A | ..406E-6 | 4.61284116 | 0.84983355 |
| | | | | B | ..376E-6 | 4.7301726 | 0.84953928 |
| 0.15 | 0.05 | | | A | .363E-6 | 4.6882911 | 0.85006821 |
| | | | | B | .415E-6 | 4.8149781 | 0.84978342 |
| 0.01 | 0.1667 | | | A | .391E-6 | 4.7519069 | 0.84999305 |
| | | | | B | .276E-6 | 4.7519069 | 0.84968738 |

Table 24

Complete Results of Best Fit Parameters of Equation T

| $b_2$ | $b_3$ | $n^*$ | $T^*$ | N | SDSS | $P^*$ | $U^*$ |
|---|---|---|---|---|---|---|---|
| -0.33 | 0.19 | 0.001 | 3.3333 | A | 0 | 1.0003558 | 0.99865645 |
|  |  |  |  | B | 0 | 1.0003558 | 0.99865717 |
|  |  | 0.10 |  | A | .193E-7 | 1.0548491 | 0.86611313 |
|  |  |  |  | B | .557E-8 | 1.0556784 | 0.86621141 |
|  |  | 0.30 |  | A | .763E-7 | 1.3419741 | 0.59225386 |
|  |  |  |  | B | .449E-7 | 1.3419741 | 0.59225386 |
|  |  | 0.50 |  | A | .188E-6 | 2.1027668 | 0.29618740 |
|  |  |  |  | B | .149E-6 | 2.1317523 | 0.29580861 |
|  |  | 0.70 |  | A | .638E-6 | 4.0193305 | -0.0063024759 |
|  |  |  |  | B | .294E-6 | 4.1982203 | -0.006194531 |
|  |  | 0.75 |  | A | .841E-6 | 4.8563266 | -0.075227857 |
|  |  |  |  | B | .764E-6 | 5.1489840 | -0.074105978 |
|  |  | 0.80 |  | A | .770E-6 | 5.905870 | -0.13865650 |
|  |  |  |  | B | .578E-6 | 6.3849936 | -0.13581800 |
|  |  | 0.85 |  | A | .187E-5 | 7.2014093 | -0.19547379 |
|  |  |  |  | B | .680E-6 | 7.9788857 | -0.18993819 |
| -1.0 | 0.4 | 0.001 | 1.8 | A | .558E-10 | 0.99840188 | -0.99678862 |
|  |  |  |  | B | 0 | 0.99840188 | -0.99679203 |
|  |  | 0.10 |  | A | .273E-8 | 0.87233138 | 0.69358087 |
|  |  |  |  | B | .187E-7 | 0.87274837 | 0.69405240 |

Table 24--Continued

| $b_2$ | $b_3$ | n* | T* | N | SDSS | P* | U* |
|---|---|---|---|---|---|---|---|
| -1.0 | 0.4 | 0.25 | 1.8 | A | .611E-7 | 0.83400637 | 0.2886990 |
| | | | | B | .703E-7 | 0.83773023 | 0.29058182 |
| | | 0.45 | | A | .112E-6 | 1.1843519 | -0.22834468 |
| | | | | B | .1E-6 | 1.2037913 | -0.22598970 |
| | | 0.60 | | A | .174E-6 | 1.8636935 | -0.63180506 |
| | | | | B | .315E-6 | 1.9043090 | -0.62928247 |
| | | 0.70 | | A | .716E-6 | 2.5572543 | -0.90043151 |
| | | | | B | .173E-5 | 2.6423690 | -0.89681387 |
| | | 0.75 | | A | .748E-6 | 3.1743598 | -1.0271902 |
| | | | | B | .106E-5 | 3.4189560 | -1.0219886 |
| | | 0.85 | | A | .242E-5 | 5.7713513 | -1.2314889 |
| | | | | B | .305E-5 | 7.1085725 | -1.2149594 |
| -0.37 | 0.17 | 0.001 | 2.6 | A | 0 | 0.99976313 | 0.99812573 |
| | | | | B | 0 | 0.9976319 | 0.99812669 |
| | | 0.10 | | A | .108E-7 | 0.99744749 | 0.81640339 |
| | | | | B | 0 | 0.99612220 | 0.81262630 |
| | | 0.30 | | A | .586E-7 | 1.1794686 | 0.45854568 |
| | | | | B | .697E-7 | 1.1842876 | 0.45912135 |
| | | 0.50 | | A | .160E-6 | 1.8469712 | 0.083524704 |
| | | | | B | .146E-6 | 1.8761592 | 0.03683372 |
| | | 0.65 | | A | .413E-6 | 2.9982064 | -0.20593274 |
| | | | | B | .477E-6 | 3.0955153 | -0.20593274 |

Table 24--Continued

| $b_2$ | $b_3$ | $n^*$ | $T^*$ | N | SDSS | $P^*$ | $U^*$ |
|---|---|---|---|---|---|---|---|
| -0.37 | 0.17 | 0.85 | 2.6 | A | .542E-5 | 6.5359292 | -0.53859425 |
| | | | | B | .561E-6 | 7.2045317 | -0.53032815 |
| 0.05 | 0.034 | 0.001 | 6.11 | A | 0 | 1.0012118 | 0.9936026 |
| | | | | B | 0 | 1.0012118 | 0.99936056 |
| | | 0.10 | | A | .217E-7 | 1.1423963 | 0.93420237 |
| | | | | B | 0 | 1.1426346 | 0.93422520 |
| | | 0.30 | | A | .715E-7 | 1.6266403 | 0.78929526 |
| | | | | B | .525E-7 | 1.6316613 | 0.78919798 |
| | | 0.50 | | A | .233E-6 | 2.6412497 | 0.62660205 |
| | | | | B | .132E-6 | 2.6749732 | 0.62507545 |
| | | 0.70 | | A | .125E-5 | 4.7733541 | 0.4609472 |
| | | | | B | .205E-5 | 4.9418039 | 0.406183 |
| | | 0.75 | | A | .279E-6 | 5.5842185 | 0.42263716 |
| | | | | B | .179E-5 | 5.8296647 | 0.42268503 |
| | | 0.80 | | A | .613E-6 | 6.5669789 | 0.38673162 |
| | | | | B | .155E-5 | 6.9303708 | 0.38749117 |
| | | 0.85 | | A | .1E-5 | 7.7274883 | 0.35369784 |
| | | | | B | .169E-5 | 8.2627125 | 0.35556686 |
| 0.026 | 0.088 | 0.001 | 10 | A | 0 | 1.0015733 | 0.99963313 |
| | | | | B | 0 | 1.0015733 | 0.99963331 |
| | | 0.10 | | A | .104E-7 | 1.1809695 | 0.96167248 |
| | | | | B | .177E-8 | 1.18122481 | 0.96167248 |

Table 24--Continued

| $b_2$ | $b_3$ | $n^*$ | $T^*$ | N | SDSS | $P^*$ | $U^*$ |
|---|---|---|---|---|---|---|---|
| 0.026 | 0.088 | 0.30 | 10 | A | .540E-7 | 1.7542067 | 0.87440532 |
|  |  |  |  | B | .621E-7 | 1.7593472 | 0.87429506 |
|  |  | 0.50 |  | A | .104E-6 | 2.8672721 | 0.77464390 |
|  |  |  |  | B | .139E-6 | 2.9022400 | 0.77421975 |
|  |  | 0.70 |  | A | .391E-6 | 5.1416540 | 0.67305988 |
|  |  |  |  | B | .539E-6 | 5.3331351 | 0.67266876 |
|  |  | 0.80 |  | A | .912E-6 | 7.0655479 | 0.62760705 |
|  |  |  |  | B | .986E-6 | 7.5034437 | 0.62787783 |
| -0.03 | 0.06 | 0.001 | 20 | A | 0 | 1.0018418 | 0.99982548 |
|  |  |  |  | B | 0 | 1.0018418 | 0.99982560 |
|  |  | 0.10 |  | A | .708E-8 | 1.2104031 | 0.98153520 |
|  |  |  |  | B | 0 | 1.2106794 | 0.98153520 |
|  |  | 0.30 |  | A | .371E-7 | 1.8480663 | 0.93843150 |
|  |  |  |  | B | .3E-7 | 1.8530670 | 0.93835747 |
|  |  | 0.45 |  | A | .670E-7 | 2.6385379 | 0.90131837 |
|  |  |  |  | B | .170E-6 | 2.6589773 | 0.90111196 |
|  |  | 0.60 |  | A | .261E-6 | 3.9071531 | 0.86220622 |
|  |  |  |  | B | .383E-6 | 3.9789257 | 0.86188108 |
|  |  | 0.75 |  | A | .379e-6 | 6.0164571 | 0.82993061 |
|  |  |  |  | B | .708E-6 | 6.2624044 | 0.82477766 |
|  |  | 0.85 |  | A | .386E-5 | 8.1883526 | 0.80352145 |
|  |  |  |  | B | .272E-5 | 8.7524891 | 0.80371943 |

# APPENDIX B

## COMPUTER PROGRAMS

This appendix lists all computer programs that were used for this study and also discusses the changes that were made for their improvements. The first thing that were done was to transfer all programs from DEC PDP 10 system to a much faster computing system, DEC VAX. The following are the procedures involved, written in point form.

1. Log-in the PDP 10 system.
2. At the monitor prompt (.) type the exactly the following,

   ```
   .R NFT
   ```

   which means 'run network file transfer'
3. When a star prompt appear (*), type exactly the following,

   ```
   *COPY POOH::MAIN8.FOR/USER:86ISMAIL=MAIN7.FOR
               new filename               old filename
   ```

4. Messages appear asking for the following informations,

   ```
   USER ID:    86ISMAIL       (Enter your VAX username)
   ACCOUNT:    <R>            (Type RETURN)
   PASSWORD:   TAQWA          (Type your secret password)
   ```

5. Messages appear to confirm that the file has completely transfered.
6. To exit type EXIT at star (*) prompt.

Note that the example shown above is the case of this particular study. A more general explaination are in the next two pages supplied by Achedemic Computer Center at Western Michigan University.

# ASCII File Transfers Between the DECsystem-10 and the VAXes

1.102
7/86-SMT

## DEC-10 ==> VAX

To transfer a file from the DECsystem-10 to the VAX you need to log onto the DEC-10 and run the program NFT (Network File Transfer) typing the following command at the DEC-10 prompt (.):

```
.R NFT
```

At the * prompt which will appear, type the COPY command (you substitute the appropriate node, device, directory and filename):

```
COPY node::device:[directory]vaxfilename/USERID=decfilename
```

The program will respond with a message and then request you to enter the following information about your VAX account:

```
USER-ID:
ACCOUNT:                (just press the RETURN key)
PASSWORD:               (will not echo password)
```

A message recounting the transfer process will appear in the following form:

```
Node::device:[directory]vaxfilename <== DSK:[ppn]decfilename
```

This will be followed by a message about the size of the file transferred and the asterisk will reappear. At this point simply enter EXIT to leave the program or enter another NFT command.

Example:

```
.R NFT

*COPY POOH::DISK$BIS:[JONES]newfil2.dat/USERID=newfil.dat

USER-ID: JONES          (VAX login username)
ACCOUNT:
PASSWORD:               (enter VAX password)

POOH::DISK$BIS:[JONES]newfil2.dat <== DSK:[ppn]newfil.dat

*EXIT
```

## VAX ===> DEC-10

To copy a file from the VAX to the DEC-10 run the NFT program on the DEC-10 (as described above) using the **R NFT** command and switch the VAX information to the other side of the "=" sign. The command can be shortened to:

```
*COPY decfilename=node::vaxfilename/USERID
```

As with the DEC-10 to VAX transfer, you will be asked for information about the VAX account.

If the VAX filename contains underscores or special characters, it must be enclosed in double quotes (") in the NFT command line. The DEC-10 file into which it is moved must have a valid DEC-10 file name.

## SIMPLIFYING THE COMMAND

If you want to simplify the **COPY** command further, you can put the following line in your SWITCH.INI file:

```
NFT/USERID:username:username
```

The **COPY** command can then be reduced to:

```
*COPY node::=decfilename                (to copy from the DEC-10 to the VAX)
```

and

```
*COPY decfilename=node::vaxfilename     (to copy from the VAX to the DEC-10)
```

## GETTING HELP

There is online help available for NFT. To read it, enter **HELP NFT** at the DEC-10 prompt (.). To obtain a printed copy of this help file enter the following command at the DEC-10 prompt:

```
PRINT HLP:NFT.HLP
```

## Warning:

Since the network attempts to login to the VAX account using the USERID and PASSWORD specified, if there are any errors in your LOGIN.COM file on the VAX, the program will fail. To prevent the processing of your LOGIN.COM file during network logins, insert the following line at the beginning of your LOGIN.COM file:

```
$IF F$MODE() .EQS. "NETWORK" THEN $EXIT
```

The main task after the transfer is to make the new system capable of understanding the command statements that appear in the program transferred. So few changes are necessary. Fortunately, the problem didn't arises when dealing with all Basic programs since both systems use the same commands. The three basic programs; the LEASTSQ.BAS, PAD.BAS QUADRATIC.BAS are listed in the next four pages. The Least square fit program basically deals with equation 37 and 38.

$$P^* = P_0^* + C_1b_2 + C_2b_3 + C_3b_2^2 + C_4b_3^2 + C_5b_2b_3 \quad (40)$$

$$U^* = U_0^* + C_1b_2 + C_2b_3 + C_3b_2^2 + C_4b_3^2 + C_5\, b_2\, b_3 \quad (41)$$

The QUADRATIC.BAS uses the same equation to compute b2 and b3 given values of $P^*$ and $P_o^*$. The PAD.BAS program is used for interpolation using formulas

$$P^* = \frac{(\ 1 + a1n^* + a2n^* + a3n^*\ )}{(\ 1 + a4n^* + a5n^* + a6n^*\ )}$$

$$U = \frac{(\ 1 + a1n^* + a2n^* + a3n^*\ )}{(\ 1 + a4n^* + a5n^* + a6n^*\ )}$$

The only program written in FORTRAN is the MAIN8 which is the improvement of MAIN7. Changes are listed in points form.

## QUADRATIC.BAS PROGRAM

```
10    REM THIS PROGRAM IS DESIGNED TO COMPUTE B2, GIVEN A
       VALUE OF B3
20    PRINT "TYPE THE PY VALUE"
30    INPUT P0
40    PRINT "TYPE THE P* OR U* VALUE"
50          FOR S = 1 TO 5
60          INPUT L
70          LET C(S) = L
80          NEXT S
90                A = -1.00
100               A = A + 0.05
110               E = ( C ( 2 ) + C ( 5 ) • A )
120               S = C ( 1 ) • A + C ( 3 ) • A • A + P0 - P
130               P1 = -( E + E/ABS ( E ) • SQRT ( E • E - 4 • C ( 4 ) • F ))/
                       ( 2 • C ( 4 ) )
140               B2 = F / ( C ( 4 ) • B1 )
150   PRINT B1, B2, A
160   IF A > 1. 00 THEN 170
165   GO TO 100
170   PRINT " DO YOU WANT TO TEST OTHER VALUE ? "
180   INPUT T
190   IF T = 3 THEN 20
200   END
```

```
    LEASTSQ.BAS
5 REM " P* = Po* + c1b2 + c2b3 + c3b2**2 + c4b3**2 + c5b2b3"
6 rem " U* = Uo* + c1b2 + c2b3 + c3b2**2 + c4b3**2 + c5b2b3"
10  DIM A(20), B(20), Y(20), X(5,5), C(5,1), Z(5,1)
15 MAT Z = ZER
20 MAT X = ZER
30 PRINT "TYPE THE NO. OF POINTS"
40 INPUT N
50 PRINT " TYPE THE PY VALUES "
60 INPUT P
70 PRINT " TYPE THE N VALUES OF P "
80 FOR J = 1 TO N
90    INPUT P1
100   Y(J) = P1 - P
110 NEXT J
120 PRINT " TYPE THE N VALUES OF A "
130 FOR J = 1 TO N
140     INPUT A(J)
150 NEXT J
160 PRINT " TYPE THE N VALUES OF B "
170 FOR J = 1 TO N
180      INPUT B(J)
190 NEXT J
200 FOR J = 1 TO N
210     X(1,1) = X(1,1) + A(J)*A(J)
220     X(1,2) = X(1,2) + A(J)*B(J)
230     X(1,3) = X(1,3) + A(J)*A(J)*A(J)
240     x(1,4) = x(1,4) + A(J)*B(J)*B(J)
250     X(1,5) = X(1,5) + A(J)*A(J)*B(J)
260     X(2,2) = X(2,2) + B(J)*B(J)
270     X(3,3) = X(3,3) + A(J)*A(J)*A(J)*A(J)
280     X(2,4) = X(2,4) + B(J)*B(J)*B(J)
290     X(3,4) = X(3,4) + A(J)*A(J)*B(J)*B(J)
295     X(5,5) = X(5,5) + A(J)*A(J)*B(J)*B(J)
300     X(3,5) = X(3,5) + A(J)*A(J)*A(J)*B(J)
310     X(4,4) = X(4,4) + B(J)*B(J)*B(J)*B(J)
320     X(4,5) = X(4,5) + A(J)*B(J)*B(J)*B(J)
330     X(2,1) = X(1,2)
340     X(2,3) = X(1,5)
350     X(2,5) = X(1,4)
360     X(3,1) = X(1,3)
370     X(3,2) = X(2,3)
380     X(4,1) = X(1,4)
390     X(4,2) = X(2,4)
400     X(4,3) = X(3,4)
410     X(5,1) = X(1,5)
420     X(5,2) = X(2,5)
430     X(5,3) = X(3,5)
440     X(5,4) = X(4,5)
```

```
450            Z(1,1) = Z(1,1) + A(J)*Y(J)
460            Z(2,1) = Z(2,1) + B(J)*Y(J)
470            Z(3,1) = Z(3,1) + A(J)*A(J)*Y(J)
480            Z(4,1) = Z(4,1) + B(J)*B(J)*Y(J)
490            Z(5,1) = Z(5,1) + A(J)*B(J)*Y(J)
495  NEXT J
500   MAT D = INV(X)
510 MAT C = D*Z
520   PRINT
530 PRINT "C1 =" ; C(1,1)
540 PRINT "C2 =" ; C(2,1)
550 PRINT "C3 =" ; C(3,1)
560 PRINT "C4 =" ; C(4,1)
570 PRINT "C5 =" ; C(5,1)
580 PRINT
590 PRINT "A","B","P", "P-CALC"
600 PRINT
610 FOR J =1 TO N
620      P1 = P + Y(J)
630 P2 = P + C(1,1)*A(J) + C(2,1)*B(J) + C(3,1)*A(J)*A(J) + C(4,1)*B(J)+
(5,1)*A(J)*B(J)
640  PRINT A(J),B(J),P1,P2
650 NEXT J
660 PRINT " DETERMINANT OF X " ,DET
670 END
```

**Pad.Bas**

```
11   dim d(6),p(6),c(6,1),a(6,1),w(6,6),b(6,6)
15   def fnb(x) = 1 + a(1,1)*x + a(2,1)*x*x + a(3,1)*x*x*x
16   def fnc(x) = 1 + a(4,1)*x + a(5,1)*x*x + a(6,1)*x*x*x
17   def fna(x) = fnb(x)/fnc(x)
20   print "type the 6 densities"
21   input d(1),d(2),d(3),d(4),d(5),d(6)
22   print "type the 6 y-values"
23   input p(1),p(2),p(3),p(4),p(5),p(6)
25   for j = 1 to 6
26   c(j,1) = p(j) - 1
27   w(j,1) = d(j)
28   w(j,2) = d(j)*d(j)
29   w(j,3) = d(j)*d(j)*d(j)
30   w(j,4) = -p(j)*d(j)
31   w(j,5) = -p(j)*d(j)*d(j)
32   w(j,6) = -p(j)*d(j)*d(j)*d(j)
33   next j
35   mat b = inv(w)
36   mat a = b*c
37   print
38   print "pade ceofficients"
39   print
40   print "a1 = ";a(1,1)
41   print "a2 = ";a(2,1)
42   print "a3 = ";a(3,1)
43   print "a4 = ";a(4,1)
44   print "a5 = ";a(5,1)
45   print "a6 = ";a(6,1)
46   print
47   print "j", "density", "input y", "output y"
48   print
49   for j = 1 to 6
50   y = fna(d(j))
51   print j,d(j),p(j),y
52   next j
55   print
56   print "type 1 to end, 2 to print values"
57   input j1
58   if j1 = 1 then 76
59   print "type initial density, interval, and number of points"
60   input d1,d2,j3
65   print
66   print "density", "y", "numerator", "denominator"
67   print
70   for j = 1 to j3
71   x = d1 + (j - 1)*d2
72   print x, fna(x), fnb(x),fnc(x)
73   next j
74   print
75   goto 56
76   end
```

| <u>LINES</u> | <u>CHANGES</u> |
|---|---|
| 1. 100, 200, 300, 400 | To make it possible to compute more than 100 values, all dimensions are changed from 100 to 300 except SINE(600) |
| 2. 800 | The format is changed to FORMAT(I,5F15.0) This is because Vax reads values from the screen monitor differently. |
| 3. 5100, 5200, 5300 | An equation is broken down to smaller parts of equations for convenience.<br>X = 2.0 * S2(J)<br>Y = X - S4(J) - S(J)<br>IF ( Y . EQ . 0.0 ) GO TO 200 |
| 4. 5600 | To avoid computing zero dominator extrapolated SE(J) is assigned with the S(J) value. Notice that this is related to 5300. |
| 5. 7600, 7900, 8100 | The following statements are inserted,<br>IF (NTIMES .GT. 0) GO TO 61<br>READ (5,60) MT, ALPHA, NTIMES<br>NTIMES = NTIMES - 1<br>These lines are to avoid typing ALPHA each time. |
| 6. 10100, 10200, 10300<br>32600 | At this subroutine, the thermodynamic function is inserted. The CALL statements are changed to, |

| | |
|---|---|
| | CALL STOG3 (S,G,BPHI,R,N,P2,P3,DEN,DEL)<br>CALL STOG3 (S2,GI,BPHI,R,N,P2,P3,DEN,DEL)<br>CALL STOG3 (SE,GE,BPHI,R,N,P2,P3,DEN,DEL)<br>Notice that P1,P2,P3,DEL,DEN are inserted. |
| 7. 10900, 11000, 15100<br>53000, 284000 | VAX uses different OPEN statement.<br>OPEN (UNIT = 20, ACCESS = 'SEQUEN-<br>-TIAL',STATUS = 'NEW',FILE = 'PRIN1')<br>The same changes are made for files, PRIN2,DASI1,DASI2,and DASI. |
| 8. 32700 - 35000 | Thermodynamic function THTSW.FOR and statement T = P1 are inserted.<br>Statements deleted are,<br>SP = 0.0<br>OPEN statements for FS.DAT<br>SP = SP + R*4*(1.0 - 2.0* R*6)* G(J)<br>G(JB) = 2.0 * G(JB + 1) - G(JB + 2)<br>G(JE) = 2.0 * G(JE - 1) - G(JE - 2) |

The program to compute thermodynamic functions P* and U* of Square-well is on next page, which is the original program. A new revised version of this program is in Main 8 under subroutine STOG3. Notice that this program is inserted in the main program to avoid the task of creating or renaming DASI files every time to run THTSW and thus, saving time. The MAIN8 program is listed in the last pages of this appendix

```
 THTSW.FOR
      DIMENSION S(300),G(300)
      SE = 0.0
      PI = 3.1415927
      WRITE(5,40)
  40  FORMAT(' TYPE  N,DEL,DEN,T,P2,P3   '/)
      READ(5,60) N,DEL,DEN,T,P2,P3
  60  FORMAT(I,5F)
      C1 = EXP(1.0/T)
      C2 = 1.0/C1
      OPEN(UNIT=21,ACCESS= SEQUENTIAL'.STATUS='OLD'.FILE='F3.DAT')
      READ(21,110)(S(J), J=2.N)
 110  FORMAT(E20.8)
      JB = 1.0/DEL + 1.005
      JE = 1.5/DEL + 1.005
      DO 150  J=JB,JE
 150  G(J) = C1*(1.0 + S(J) + P2*S(J)*S(J)  + P3*S(J)*S(J)*S(J))
      DO 210   J=JB,JE
      AJ = J-1
      X = AJ * DEL
 210  SE = SE + G(J)*X*X
      SE = SE - 0.5*G(JB) - 0.5*G(JE)*1.5*1.5
      E = 1.0 - (4.0*PI*DEN*DEL*SE)/(3.0*T)
      P = 1.0+((2.0*PI*DEN)/3.0)*(G(JB)-3.375*G(JE)*(1.0-C2))
      WRITE (5,260)P,E
 260  FORMAT(2E20.8)
      STOP
      END
```

MAIN8 program

```
      DIMENSION SINE(600),R(300),SI(300),BPHI(300),C(300)
      DIMENSION TC(300),S(300),S1(300),S2(300),SDSS(300),SDEE(300)
      DIMENSION SDSE(300),SE(300),G(300),GE(300),SE1(300),G1(300)
      DIMENSION S3(300),S4(300)
      WRITE(5,1)
  1   FORMAT(' TYPE N,DEL,P1,P2,P3,DEN'/)
  2   READ(5,3)N,DEL,P1,P2,P3,DEN
  3   FORMAT(I,5F)
  4   WRITE(5,5)
  5   FORMAT(' TYPE NFGS,NPON,NEQ,ALPHA'/)
  6   READ(5,7)NFGS,NPON,NEQ,ALPHA
  7   FORMAT(3I,F)
  8   NCOM = 50
  9   PI = 3.1415927
 10   RHO = (2.0*PI)**3*DEN
      IF(NFGS.GT.1) GO TO 13
      RHOC = RHO
      RHO = RHO*0.1
 13   GO TO (14,16),NFGS
 14   CALL FGS1(SI,N)
 15   GO TO 17
 16   CALL FGS2(SI,N)
 17   CONTINUE
 18   IND = 0
 19   NT= 0
 20   NDENOM = 0
 22   AN = N
 23   EL = 2.0*(AN - 1.0)*DEL
 24   C1 = EL**2/(4.0*PI**3*(2.0*AN - 1.0))
 25   C2 = 16.0*PI**3/(DEL*EL**2)
 26   CALL TRIG1(N,SINE)
 27   DO 29  J = 2,N
 28   AJ = J - 1
 29   R(J) = AJ*DEL

 30   GO TO (31,33,35),NPON
 31   CALL PONTL1(P1,P2,P3,R,N,BPHI)
 32   GO TO 36
 33   CALL PONTL2(P1,P2,P3,R,N,BPHI)
 34   GO TO 36
 35   CALL PONTL3(P1,P2,P3,R,N,BPHI)
 36   CALL ITER(SI,BPHI,R,N,SINE,TC,C1,RHO,NDENOM,
    1    S,C2,C,NEQ,P2,P3)
 37   IND = IND + 1
      IF(NFGS.GT.1) GO TO 38
      IF (IND.GT.9) GO TO 38
      AIND = IND + 1
      RHO = RHOC*(AIND/10.0)
 38   CALL RMS(SI,S,N,SD)
 39   SDSS(IND) = SD
 40   DO 41  J = 2,N
       X=2.0 *S1(J)
       Y=X-S2(J)-S(J)
        IF (Y .EQ. 0.0) GO TO 200
       SE(J) = (S1(J)**2 - S2(J)*S(J))/(2.0*S1(J) - S2(J) - S(J))
        GO TO 41
200      SE(J) = S(J)
 41    CONTINUE
 42   CALL RMS(SE,SE1,N,SD)
 43   SDEE(IND) = SD
```

```
  44    CALL RMS(SE,S,N,SD)
  45    SDSE(IND) = SD
  46    DO 49  J = 2,N
  47    S2(J) = S1(J)
  48    S1(J) = S(J)
  49    SE1(J) = SE(J)
  50    IF(NDENOM)53,53,51
  51    WRITE(5,52)
  52    FORMAT( 'DENOMINATOR WENT NEGATIVE')
        NDENOM = 0
  53    WRITE(5,54)
  54    FORMAT( '  ITER              SDSS            SDSE            SDEE    '/)
  55    WRITE(5,56)IND,SDSS(IND),SDSE(IND),SDEE(IND)
  56    FORMAT(I5,E15.3,2E12.3)
  57    IF (NTIMES .GT. 0) GO TO 61
         WRITE(5,58)
  58    FORMAT(' TYPE 1.CONT,2.EXT,3.ABORT,4.FIN,5.GOBACK:ALPHA,NTIMES'/)
  59    READ(5,60)MT,ALPHA,NTIMES
  60    FORMAT(I,F)
  61    NTIMES=NTIMES-1
        GO TO (62,65,157,74,68),MT
  62    DO 63  J=2,N
  63    SI(J)=S(J)*ALPHA + (1.0-ALPHA)*SI(J)
  64    GO TO 36
  65    DO 66  J=2,N
  66    SI(J) = SE(J)
  67    GO TO 36
  68    DO 69  J = 2,N
  69    SI(J) = S2(J)
  70    GO TO 36
  74    GO TO (75,79,83,87),NEQ
  75    CALL STOG1(S,G,RPHI,R,N)
  76    CALL STOG1(S2,G1,RPHI,R,N)
  77    CALL STOG1(SE,GE,RPHI,R,N)
  78    GO TO 90
  79    CALL STOG2(S,G,RPHI,R,N)
  80    CALL STOG2(S2,G1,RPHI,R,N)
  81    CALL STOG2(SE,GE,RPHI,R,N)
  82    GO TO 90
  83    CALL STOG3(S,G,RPHI,R,N,P1,P2,P3,DEN,DEL)
  84    CALL STOG3(S2,G1,RPHI,R,N,P1,P2,P3,DEN,DEL)
  85    CALL STOG3(SE,GE,RPHI,R,N,P1,P2,P3,DEN,DEL)
  86    GO TO 90
  87    CALL STOG4(S,G,RPHI,R,N,P3,APAR)
  88    CALL STOG4(S2,G1,RPHI,R,N,P3,APAR)
  89    CALL STOG4(SE,GE,RPHI,R,N,P3,APAR)
  90    IF(NT)1091,1091,1093
1091    OPEN (UNIT=20,ACCESS='SEQUENTIAL',STATUS='NEW',FILE='PRIN1')
1092    GO TO 1090
1093    OPEN (UNIT=20,ACCESS='SEQUENTIAL',STATUS='NEW',FILE='PRIN2')
1090    WRITE(20,91)
  91    FORMAT(44H1 RADIAL DISTRIBUTION FUNCTION GENERAL CODE       )
  92    WRITE(20,93)
  93    FORMAT(26H  DC CARLEY  PHYSICS DEPT    )
1094     WRITE(20,1095)NPON,NEQ
1095    FORMAT(10H    NPON=  I10,9H   NEQ=  I10)
  94    WRITE(20,95)
  95    FORMAT(21H  POTENTIAL FUNCTION  //)
  96    WRITE(20,97)
  97    FORMAT(13H  RUN NUMBER  //)
```

```
  98   WRITE(20,99)
  99   FORMAT(30H  DIRECT CORRELATION FUNCTION  //)
 100   WRITE(20,101)ALPHA,DEN,P1,P2,P3
 101   FORMAT(10H  ALPHA = F5.3,15H     DENSITY =  F7.4,10H     P1 =
    1    E10.4,10H      P2 =  E10.4,10H      P3 =  E10.4 ///)
 102   WRITE(20,103)
 103   FORMAT(41H ITERATION            RMS(S-S)       RMS(S-SE)
    1  15H       RMS(SE-SE) //)
 104   WRITE(20,105)(J,SDSS(J),SDSE(J),SDEE(J),  J=1,IND)
 105   FORMAT(I6,E20.4,2E15.4)
 106   WRITE(20,91)
 107   WRITE(20,93)
 108   WRITE(20,109)
 109   FORMAT(50H          R               S1              SE            S
    1    59H            G1              GE             G                C
    2    14H       TC      J               //)
 110   DO 117   J = 2,N
 111   WRITE(20,112)R(J),S2(J),SE(J),S(J),G1(J),GE(J),G(J),C(J),TC(J),J
 112   FORMAT(F8.4,3E14.5,3F15.5,E14.5,E10.2,I4)
 113   IF(J - NCOM) 117,114,117
 114   NCOM = NCOM + 50
 115   WRITE(20,116)
 116   FORMAT(48H1      R               S1              SE            S
    1    59H              G1              GE             G               C
    2    15H         TC      J      //)
 117   CONTINUE
       CLOSE (UNIT=20)
 118   IF(NPUN) 121,119,121
 119   IF(NT)1190,1190,1192
1190   OPEN (UNIT=20,ACCESS='SEQUENTIAL',STATUS='NEW',FILE='DASI1')
1191   GO TO 1193
1192   OPEN (UNIT=20,ACCESS='SEQUENTIAL',STATUS='NEW',FILE='DASI2')
1193   WRITE(20,120)(S(J),J=2,N)
 120   FORMAT(E20.8)
       CLOSE (UNIT=20)
 121   CONTINUE
       WRITE(5,122)
 122   FORMAT(' TYPE 1 TO FIN,2 TOEXT RAN,3 TO 2XN,4 TO 4XN;N'/)
 123   READ(5,124)NT,N
 124   FORMAT(2I)
 125   GO TO(157,22,128,140),NT
 128   N = 2*N - 1
 130   DO 132   J = 3,N,2
 131   K = J/2 + 1
 132   SI(J) = S(K)
 133   DO 135   J = 4,N,2
 134   K = J/2
 135   SI(J) = 0.5*(S(K) + S(K + 1))
 136   SI(2) = 2.0*SI(3) - SI(4)
 137   DEL = DEL*0.5
 139   GO TO 22
 140   N = 4*N - 3
 142   DEL = DEL*0.250
 143   DO 145   J = 5,N,4
 144   K = J/4 + 1
 145   SI(J) = S(K)
 146   DO 149   J = 7,N,4
 147   K = J/4 + 1
 148   SI(J) = 0.5*(S(K) + S(K + 1))
 149   DO 150   J = 6,N,4
```

```
150   SI(J) = 0.5*(SI(J - 1) + SI(J + 1))
151   DO 152  J = 8,N,4
152   SI(J) = 0.5*(SI(J - 1) + SI(J + 1))
153   SI(4) = 2.0*SI(5) - SI(6)
154   SI(3) = 2.0*SI(4) - SI(5)
155   SI(2) = 2.0*SI(3) - SI(4)
156   GO TO 22
157   CALL EXIT
      END
      SUBROUTINE ITER(SI,BPHI,R,N,SINE,TC,C1,RHO,NDENOM,SOUT,
   1   C2,C,NEQ,P2,P3)
      DIMENSION SI(300),BPHI(300),R(300),C(300),SINE(600),TC(300)
      DIMENSION TS(300),SOUT(300)
  3   GO TO (4,6,8,10),NEQ
  4   CALL DC1(SI,BPHI,R,N,C)
  5   GO TO 11
  6   CALL DC2(SI,BPHI,R,N,C)
  7   GO TO 11
  8   CALL DC3(SI,BPHI,R,N,C,P2,P3)
  9   GO TO 11
 10   CALL DC4(SI,BPHI,R,N,C,P2,P3)
 11   CONTINUE
 12   CALL FOURTR(N,SINE,C,TC,R,C1)
 13   NDENOM = 0
 14   DO 20  K = 2,N
 15   ANUM = RHO*TC(K)**2
 16   DENOM = 1.0 - RHO*TC(K)
 17   TS(K) = ANUM/DENOM
 18   IF (DENOM) 19,19,20
 19   NDENOM = 1
 20   CONTINUE
 21   CALL INVSTR(N,SINE,TS,SOUT,C2)
 22   RETURN
      END
      SUBROUTINE PONTL1(P1,P2,P3,R,N,BPHI)
      DIMENSION R(300),BPHI(300)
  3   DO 8  J = 2,N
  4   IF (R(J) - 1.0) 5,5,7
  5   BPHI(J) = 1.0E+20
  6   GO TO 8
  7   BPHI(J) = 0.0
  8   CONTINUE
  9   K = 1.0/(R(2) - R(1)) + 1.005
 10   BPHI(K) = 0.69315
 11   RETURN
      END
      SUBROUTINE RMS(A,B,M,SD)
      DIMENSION A(300),B(300)
  3   SUM = 0.0
  4   DO 5  J = 2,M
  5   SUM = SUM + (A(J) - B(J))**2
  6   AM = M
  7   SD = SQRT(SUM/AM)
  8   RETURN
      END
      SUBROUTINE FOURTR(N,SINE,A,TA,R,C1)
      DIMENSION SINE(600),A(300),TA(300),R(300),RA(300)
  3   DO 4  J = 2,N
  4   RA(J) = R(J)*A(J)
  5   DO 15  K = 2,N
```

```
SUM = 0.0
KN = K
DO 13  J = 2,N
SUM = SUM + RA(J)*SINE(KN)
KN = KN + K - 1
IF (KN - (2*N - 1)) 13,13,12
KN = KN - (2*N - 1)
CONTINUE
AK = K - 1
TA(K) = C1*SUM/AK
RETURN
END
SUBROUTINE INVSTR(N,SINE,TA,A,C2)
DIMENSION SINE(500),A(300),TA(300),TAK(300)
DO 5  K = 2,N
AK = K - 1
TAK(K) = TA(K)*AK
DO 16  J = 2,N
SUM = 0.0
JN = J
DO 14  K = 2,N
SUM = SUM + TAK(K)*SINE(JN)
JN = JN + J - 1
IF (JN - (2*N - 1)) 14,14,13
JN = JN - (2*N - 1)
CONTINUE
AJ = J - 1
A(J) = C2*SUM/AJ
RETURN
END
SUBROUTINE FGS1(SI,N)
DIMENSION SI(300)
DO 4  J = 1,N
SI(J) = 0.0
RETURN
END
SUBROUTINE FGS2(SI,N)
DIMENSION SI(300)
OPEN (UNIT=21,ACCESS='SEQUENTIAL',STATUS='OLD',FILE='DASI')
READ(21,5)(SI(J),J = 2,N)
FORMAT(E20.8)
RETURN
END
SUBROUTINE TRIG1(N,SINE)
DIMENSION SINE(500)
M = 2*N - 1
AM = M
C = 2.0*3.14159/AM
DO 8  J = 1,M
AJ = J - 1
SINE(J) = SIN(AJ*C)
RETURN
END
SUBROUTINE STOG1(S,G,BPHI,R,N)
DIMENSION S(300),G(300),BPHI(300),R(300)
DO 4  J = 2,N
G(J) = (S(J) + 1.0)*EXP(-BPHI(J))
RETURN
END
SUBROUTINE STOG2(S,G,BPHI,R,N)
```

```
      DIMENSION S(300),G(300),BPHI(300),R(300)
  3   DO 4  J = 2,N
  4   G(J) = EXP(S(J) - BPHI(J))
  5   RETURN
      END
      SUBROUTINE DC1(SG,BPHI,R,N,C)
      DIMENSION SG(300),BPHI(300),R(300),C(300)
  3   DO 4  J = 2,N
  4   C(J) = (SG(J) + 1.0)*(EXP(-BPHI(J)) - 1.0)
  5   RETURN
      END
      SUBROUTINE DC2(SG,BPHI,R,N,C)
      DIMENSION SG(300),BPHI(300),R(300),C(300)
  3   DO 4  J = 2,N
  4   C(J) = EXP (SG(J) - BPHI(J)) - SG(J) - 1.0
  5   RETURN
      END
      SUBROUTINE DC3(SG,BPHI,R,N,C,P2,P3)
      DIMENSION SG(300),BPHI(300),R(300),C(300)
  3   DO 4  J = 2,N
  4   C(J) = (1.0+SG(J)+P2*SG(J)*SG(J)+P3*SG(J)*SG(J)*SG(J))*EXP
     1     (-BPHI(J))-1.0-SG(J)
  5   RETURN
      END
      SUBROUTINE STCG3(S,G,BPHI,R,N,P1,P2,P3,DEN,DEL)
      DIMENSION S(300),G(300),BPHI(300),R(300)
      T = P1
      SE = 0.0
      PI = 3.1415927
      C1 = EXP(1.0/T)
      C2 = 1.0/C1
      JB = 1.0/DEL + 1.005
      JE = 1.5/DEL + 1.005
      DO 150  J = JB,JE
150     G(J)=(1.0+S(J)+P2*S(J)*S(J)+P3*S(J)*S(J)*S(J))*C1
       DO 210  J = JB,JE
       AJ = J - 1
        X = AJ*DEL
210       SE = SE + G(J)*X*X
       SE = SE - 0.5*G(JB)- 0.5*G(JE)*1.5*1.5
       E = 1.0 - (4.0*PI*DEN*DEL*SE)/(3.0*T)
       P = 1.0 + ((2.0*PI*DEN)/3.0)*(G(JB) - 3.375*G(JE)*(1.0 - C2))
       WRITE(5,260)P,E
260       FORMAT(2E20.8)
      RETURN

      END
      SUBROUTINE PONTL2(P1,P2,P3,R,N,BPHI)
      DIMENSION R(300),BPHI(300)
  3   DO 11  J=2,N
  4   IF (R(J) - 1.0) 5,5,7
  5   BPHI(J) = 1.0E+20
  6   GO TO 11
  7   IF (R(J) - 1.5) 8,8,10
  8   BPHI(J) = -(1.0/P1)
  9   GO TO 11
 10   BPHI(J) = 0.0
 11   CONTINUE
 12   K1 = 1.0/(R(2) - R(1)) + 1.005
 13   K2 = 1.5/(R(2) - R(1)) + 1.005
```

```
14    BPHI(K1) = 0.69315 - 1.0/P1
15    BPHI(K2) = -ALOG(0.5 + 0.5*EXP(1.0/P1))
16    RETURN
      END
      SUBROUTINE PONTL3(P1,P2,P3,R,N,BPHI)
      DIMENSION R(300),BPHI(300)
 3    DO 6  J = 2,N
 4    X = (1.0/R(J))**6
 5    X2 = X**2
 6    BPHI(J) = 4.0*(X2 - X)/P1
 7    RETURN
      END
      SUBROUTINE DC4(SG,BPHI,R,N,C,P2,P3)
      DIMENSION SG(300),BPHI(300),R(300),C(300)
 3    DO 4  J = 2,N
 4    C(J) = EXP(-BPHI(J))*(1.0-1.0/P3+EXP(P3*SG(J))/P3)-SG(J)-1.0
 5    RETURN
      END
      SUBROUTINE STOG4(S,G,BPHI,R,N,P2,P3)
      DIMENSION S(300),G(300),BPHI(300),R(300)
 3    DO 4  J = 2,N
 4    G(J) = EXP(-BPHI(J))*(1.0-1.0/P3+EXP(P3*S(J))/P3   )
 5    RETURN
      END
```

# APPENDIX C

## DERIVATION OF THERMODYANAMIC EQUATION

This appendix shows the derivations of $P^*$ and $U^*$ equation of state from general (equation 16 and 18) to the specific case of our study (equation 17 and 19).

The potential function for square-well,

$$ø(r) = \begin{cases} \infty & r < d \\ - & d \leq r \leq Kd \\ 0 & Kd \leq r \leq \infty \end{cases}$$

when we take $K = 1.5$

$x = r/d$

$T^* = kT/\epsilon$

$n^* = \bar{n}\, d^3$

the function becomes,

$$ø(r) = \begin{cases} \infty & x < 1 \\ -1/T^* & 1 \leq x \leq 1.5 \\ 0 & 1.5 \leq x \leq \infty \end{cases}$$

The pressure equation of state is,

$$P^* = \frac{P}{nkT} = 1 - \frac{2\pi\bar{n}}{3kT}\int_0^\infty \left(\frac{d\phi(r)}{dr}\right) g(r)\, r^3\, dr$$

$$= 1 - \frac{2\pi\bar{n}}{3kT}\int_0^\infty \left(\frac{1}{d}\right)\left(\frac{d\phi(x)}{dx}\right) g(x)\, d^4 x^3\, dx$$

$$= 1 - \frac{2\pi\bar{n}^*}{3kT}\int_0^\infty \left(\frac{d\phi}{dx}\right) g(x)\, d^4\, x^3\, dx$$

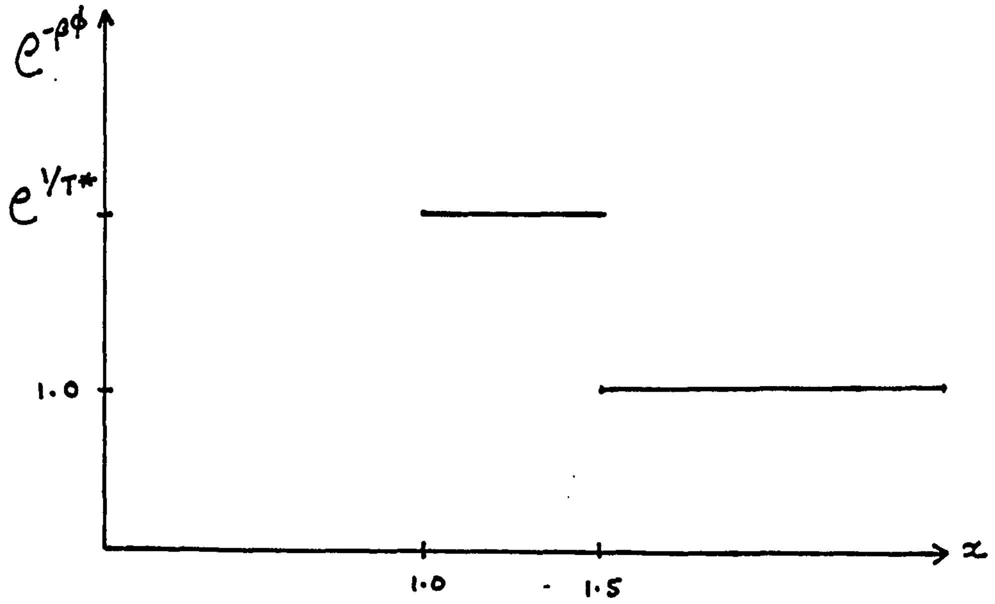
$$\frac{d}{dx}\left(e^{-\beta\phi}\right) = e^{-\beta\phi}(-\beta)\,\frac{d\phi}{dx}$$

or $$\frac{d\phi}{dx} = -kTe^{\beta\phi}\,\frac{d}{dx}\left(e^{-\beta\phi}\right)$$

$$P^* = 1 + 2\pi\bar{n}^*\int_0^\infty g(x)\, x^3 e^{\beta\phi(x)}\,\frac{d}{dx}\left(e^{-\beta\phi}\right) dx$$

$$\Psi(x) = \frac{d}{dx}\left(e^{-\beta\phi}\right)$$

Graph of $e^{-\beta\phi}$ versus x is shown in figure below,



As shown in the figure,

$\psi$ (x) = 0 except at x = 1.0 and 1.5

$\psi$ (x) = ∞

$\psi$ (x) = ∞

$$\int_{x=1.0^-}^{1.0+} \psi(x)\,dx = \left[e^{-\beta\phi}\right]_{1.0^-}^{1.0^+} = e^{1/T*}$$

$$\int_{x=1.5^-}^{1.5^+} \psi(x)\,dx = e^{-\beta\phi}\Big]_{1.5^-}^{1.5^+} = 1.0 - e^{1/T*}$$

$$\therefore \psi(x) = e^{1/T^*}\,\delta(x-1) + (1.0 - e^{1/T^*})\,\delta(x-1.5)$$

$$P^* = 1 + \frac{2\pi n^*}{3}\int_0^\infty g(x)\, e^{\beta\phi(x)}\, x^3 \left[e^{1/T^*}\delta(x-1) + (1.0 - e^{1/T^*})\,\delta(x-1.5)\right] dx$$

$$P^* = 1 + \frac{2\pi n^*}{3}\left[g(1^+)\, e^{-1/T^*} + g(1.5)\, e^{-1/T^*} (1.5)^3 (1.0 - e^{1/T^*})\right]$$

$$\boxed{P^* = 1 + \frac{2\pi n^*}{3}\left[g(1^+) - g(1.5)(1.5)^3\left\{1 - e^{-1/T^*}\right\}\right]}$$

**Internal Energy Equation of State,**

$$U^* = \frac{U}{3/2\,NkT} = 1 + \frac{4\pi N}{3VkT}\int_0^\infty \phi\, g\, r^2\, dr$$

$$= 1 + \frac{4\pi \bar{n} d^3}{3}\int_{1.0}^{1.5}\left(-\frac{1}{T^*}\right) g(x)\, x^2\, dx$$

$$\boxed{U^* = 1 - \frac{4\pi \bar{n}^*}{3T^*}\int_{1.0}^{1.5} g(x)\, x^2\, dx}$$

**Pressure and Energy at low density**

**For low density,**

$$g\,e^{\beta\phi} = 1 \quad \text{or} \quad g\,e^{-\beta\phi}$$

$$P^* = 1 + 2\pi n^* \left[ g(1^+) - g(1.5^-)(1.5)^3 \left\{ 1 - e^{-1/T^*} \right\} \right]$$

$$= 1 + \frac{2\pi n^*}{3} \left[ 1^{1/T^*} - e^{1/T^*}(1.5)^3 \left\{ 1 - e^{-1/T^*} \right\} \right]$$

$$\boxed{P^* = 1 + \frac{2\pi n^*}{3} \left[ e^{1/T^*} - 3.375\, e^{1/T^*} + 3.375 \right]}$$

If we write: $P^* = 1 + b_2 \bar{n}^* + b_3 \bar{n}^{*2} + \ldots$

$$b_2 = \left(\frac{2\pi}{3}\right) \left[ 3.375 - 2.375\, e^{1/T^*} \right]$$

$$b_2 = 2.094351 \left[ 3.375 - 2.375\, e^{1/T^*} \right]$$

$$U^* = 1 - \frac{4\pi \bar{n}^*}{3T^*} \int_1^{1.5} g(x)\, x^2\, dx$$

$$U^* \Rightarrow 1 - \frac{4\pi \bar{n}^*}{3T^*} \int_1^{1.5} e^{1/T^*} x^2 \, dx$$

$$= 1 - 4\pi \bar{n}^* e^{-1/T^*} \left[ \frac{x^3}{3} \right]_1^{1.5}$$

$$= 1 - \frac{4\pi \bar{n}^* e^{1/T^*}}{9T^*} \left[ 3.375 - 1 \right]$$

$$\boxed{U^* = 1 - (3.31625579) \left( \frac{e^{1/T^*}}{T^*} \right) \bar{n}^*}$$

$$U^* = 1 + b_2 \bar{n}^* + b_3 \bar{n}^{*2} + \ldots$$

$$\boxed{b_2 = -3.316125579 \left( \frac{e^{1/T^*}}{T^*} \right)}$$

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