Density Functional Formalism: I. Finite Temperature Theory. II. An 'Atom' in a Hot, Dense Plasma.

Uday Gupta
Louisiana State University and Agricultural & Mechanical College

Follow this and additional works at: https://digitalcommons.lsu.edu/gradschool_disstheses

Recommended Citation
https://digitalcommons.lsu.edu/gradschool_disstheses/3685

This Dissertation is brought to you for free and open access by the Graduate School at LSU Digital Commons. It has been accepted for inclusion in LSU Historical Dissertations and Theses by an authorized administrator of LSU Digital Commons. For more information, please contact gradetd@lsu.edu.
INFORMATION TO USERS

This was produced from a copy of a document sent to us for microfilming. While the most advanced technological means to photograph and reproduce this document have been used, the quality is heavily dependent upon the quality of the material submitted.

The following explanation of techniques is provided to help you understand markings or notations which may appear on this reproduction.

1. The sign or "target" for pages apparently lacking from the document photographed is "Missing Page(s)". If it was possible to obtain the missing page(s) or section, they are spliced into the film along with adjacent pages. This may have necessitated cutting through an image and duplicating adjacent pages to assure you of complete continuity.

2. When an image on the film is obliterated with a round black mark it is an indication that the film inspector noticed either blurred copy because of movement during exposure, or duplicate copy. Unless we meant to delete copyrighted materials that should not have been filmed, you will find a good image of the page in the adjacent frame. If copyrighted materials were deleted you will find a target note listing the pages in the adjacent frame.

3. When a map, drawing or chart, etc., is part of the material being photographed the photographer has followed a definite method in "sectioning" the material. It is customary to begin filming at the upper left hand corner of a large sheet and to continue from left to right in equal sections with small overlaps. If necessary, sectioning is continued again—beginning below the first row and continuing on until complete.

4. For any illustrations that cannot be reproduced satisfactorily by xerography, photographic prints can be purchased at additional cost and tipped into your xerographic copy. Requests can be made to our Dissertations Customer Services Department.

5. Some pages in any document may have indistinct print. In all cases we have filmed the best available copy.

University
Microfilms
International

300 N. ZEEB RD., ANN ARBOR, MI 48106

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
Gupta, Uday

DENSITY FUNCTIONAL FORMALISM: I. FINITE TEMPERATURE THEORY. II. AN 'ATOM' IN A HOT, DENSE PLASMA

The Louisiana State University and Agricultural and Mechanical Col. Ph.D. 1981

University Microfilms International 300 N. Zeeb Road, Ann Arbor, MI 48106

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
DENSITY FUNCTIONAL FORMALISM:
I. Finite Temperature Theory
II. An 'Atom' in a Hot, Dense Plasma

A Dissertation
Submitted to the Graduate Faculty of the Louisiana State University and Agricultural and Mechanical College in partial fulfillment of the requirements for the degree of Doctor of Philosophy in The Department of Physics and Astronomy

by
Uday Gupta

B.Sc., Calcutta University, 1970
M.Sc., Indian Institute of Technology (Kharagpur), 1973
M.S., Carnegie-Mellon University, 1976

December 1981

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
ACKNOWLEDGEMENTS

I thank Professor A. K. Rajagopal for initiating me into this area of Physics research and for his support, supervision, and guidance during the course of the work. I enjoyed working on these problems and numerous fruitful discussions with him. It is a pleasure to acknowledge Professor R. J. W. Henry for providing his Numerov computer program and for his collaboration in a part of this work. I am deeply indebted to Dr. D. A. Liberman of Los Alamos National Laboratory for providing useful numerical data and for his interest in this work. My special thanks to graduate student Yasuo Namba for his help in the cubic spline fitting program.

In addition, I appreciate the good will and support of several faculty members and students at LSU, particular Professors R. E. Miles, J. Callaway, R. O'Connell, A. R. P. Rau, and graduate students Diola Bagayoko, Mahadev Bannerjee, Calvin Countee, Arun Chatterjee, and Samir Bhattacharya.

It is a pleasure to thank Mrs. Linda Gauthier for typing this manuscript and Ms. Nancy Harris for drawing the figures. I acknowledge the Systems Network Computer Center (SNCC) for the computer facilities provided. I would like to acknowledge the travel grant of the Graduate School, Louisiana State University, for making
it possible for me to attend the 1976 NATO Summer Institute in Orleans-la-Source, France.

Finally, I would like to thank my parents for their support and understanding and many friends in Baton Rouge and elsewhere in the United States.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACKNOWLEDGEMENTS</td>
<td>ii</td>
</tr>
<tr>
<td>LIST OF TABLES</td>
<td>v</td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td>viii</td>
</tr>
<tr>
<td>ABSTRACT</td>
<td>x</td>
</tr>
<tr>
<td>CHAPTER I. Introduction</td>
<td>1</td>
</tr>
<tr>
<td>CHAPTER II. Electron Screening Effects at Finite Temperatures</td>
<td>15</td>
</tr>
<tr>
<td>I. The Effective Screened Potential</td>
<td>17</td>
</tr>
<tr>
<td>II. Ground State Energy--A Variational Calculation</td>
<td>26</td>
</tr>
<tr>
<td>III. Bound State Spectrum Due to ( V_{\text{eff}} ) Neon Impurity in Dense, Hot Plasmas</td>
<td>30</td>
</tr>
<tr>
<td>IV. Screening of Impurity States in a Semiconductor</td>
<td>37</td>
</tr>
<tr>
<td>CHAPTER III. Exchange Effects for Electron Systems at Finite Temperatures</td>
<td>45</td>
</tr>
<tr>
<td>CHAPTER IV. Electron Correlations at Finite Temperatures</td>
<td>55</td>
</tr>
<tr>
<td>CHAPTER V. The Exchange-Correlation Potential: An Application</td>
<td>72</td>
</tr>
<tr>
<td>CHAPTER VI. Summary and Concluding Remarks</td>
<td>77</td>
</tr>
<tr>
<td>REFERENCES</td>
<td>85</td>
</tr>
<tr>
<td>TABLES</td>
<td>89</td>
</tr>
<tr>
<td>FIGURES</td>
<td>112</td>
</tr>
<tr>
<td>TABLE CAPTIONS</td>
<td>127</td>
</tr>
<tr>
<td>FIGURE CAPTIONS</td>
<td>131</td>
</tr>
<tr>
<td>APPENDICES: A. First Order Exchange Integral in Classical Limit</td>
<td>135</td>
</tr>
<tr>
<td>B. Second Order Exchange Contribution</td>
<td>137</td>
</tr>
<tr>
<td>VITA</td>
<td>140</td>
</tr>
</tbody>
</table>

iv

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a.</td>
<td>Variation of Fermi Temperature ( T_F ) with Electron Density.</td>
<td>89</td>
</tr>
<tr>
<td>1b.</td>
<td>Typical Electron Densities and Temperatures of Physical Systems of Interest.</td>
<td>90</td>
</tr>
<tr>
<td>2.</td>
<td>Screening parameter ( \xi ) and Degeneracy Parameter ( a ) as a Function of ( t = T/T_F ).</td>
<td>91</td>
</tr>
<tr>
<td>3.</td>
<td>Ground State Energies for a Singly Charged Impurity in a Dense, Hot Plasma.</td>
<td>92</td>
</tr>
<tr>
<td>4.</td>
<td>Bound State Spectrum Due to a Neon Impurity in a Dense Plasma at ( T = 100 ) eV.</td>
<td>93</td>
</tr>
<tr>
<td>5.</td>
<td>The Same Neon Spectrum as in Table 4 at ( T = 750 ) eV.</td>
<td>94</td>
</tr>
<tr>
<td>5a.</td>
<td>Neon Lyman-( \alpha ) Line Shifts Obtained from Different Screening Models.</td>
<td>95</td>
</tr>
<tr>
<td>5b.</td>
<td>Breaking of Coulomb Degeneracy ( \Delta E_{2s-2p} ) Obtained from Different Screening Models.</td>
<td>96</td>
</tr>
<tr>
<td>6.</td>
<td>Neon Spectrum Obtained Using the New Ion-Sphere Potential Discussed in the Text.</td>
<td>97</td>
</tr>
<tr>
<td>7.</td>
<td>Bound State Spectrum Due to a Singly Charged Impurity in an Electron Gas at Room Temperature.</td>
<td>98</td>
</tr>
<tr>
<td>8.</td>
<td>Bound State Spectrum of a Singly Charged Donor Impurity in Silicon at Room Temperature.</td>
<td>99</td>
</tr>
<tr>
<td>Table</td>
<td>Page</td>
<td></td>
</tr>
<tr>
<td>---------</td>
<td>------</td>
<td></td>
</tr>
<tr>
<td>9.</td>
<td>100</td>
<td></td>
</tr>
</tbody>
</table>
| Exchange Energy and Exchange Potential  
Scaled by Their Respective Zero Temperature Value as a Function of \( t \) | 100  |
| 10a.    | 101  |
| Values of Exchange Energy/Particle and  
Exchange Potential as a Function of \( t \) for  
Electron Densities \( 10^{26} \) \( \text{cm}^{-3} \) | 101  |
| 10b.    | 102  |
| Values of Exchange Energy/Particle and  
Exchange Potential as a Function of \( t \) for  
Electron Densities \( 10^{24} \) \( \text{cm}^{-3} \) | 102  |
| 10c.    | 103  |
| Values of Exchange Energy/Particle and  
Exchange Potential as a Function of \( t \) for  
Electron Densities \( 10^{22} \) \( \text{cm}^{-3} \) | 103  |
| 10d.    | 104  |
| Values of Exchange Energy/Particle and  
Exchange Potential as a Function of \( t \) for  
Electron Densities \( 10^{18} \) \( \text{cm}^{-3} \) | 104  |
| 11.     | 105  |
| The Non-Interacting Part of the Thermo-  
dynamic Potential as a Function of \( t \) | 105  |
| 12a.    | 106  |
| Values of Exchange-Correlation Energies and  
Potentials as a Function of \( t \) for Electron  
Densities \( 10^{26} \) \( \text{cm}^{-3} \) | 106  |
| 12b.    | 107  |
| Values of Exchange-Correlation Energies and  
Potentials as a Function of \( t \) for Electron  
Densities \( 10^{24} \) \( \text{cm}^{-3} \) | 107  |
Table                                      Page
12c. Values of Exchange-Correlation Energies and
     Potentials as a Function of t for Electron
     Densities $10^{22} \text{ cm}^{-3}$ .................. 108
12d. Values of Exchange-Correlation Energies and
     Potentials as a Function of t for Electron
     Densities $10^{18} \text{ cm}^{-3}$ .................. 109
13. Neon Spectrum in a Dense, Hot Plasma ...... 110
14. Displaced Electron Density at the Site of a
     Proton Embedded in a Dense, Hot Plasma:
     Self-Consistent L.D.A. Calculation by Perrot
     Compared to Linear Screening Results .... 111
LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Variation of $\xi^2/\xi_{TF}^2$ and $\mu/E_F$ with $t$.</td>
<td>112</td>
</tr>
<tr>
<td>2.</td>
<td>The Effective Potential and the Associated Ground-State Form Factors in Momentum Space.</td>
<td>113</td>
</tr>
<tr>
<td>3a.</td>
<td>The Effective Potential in $r$-space Compared to Corresponding S.S.C.P.'s for Electron Density $= 4.54 \times 10^{24}$ cm$^{-3}$; $T = 100$ eV.</td>
<td>114</td>
</tr>
<tr>
<td>3b.</td>
<td>The Effective Potential in $r$-space Compared to Corresponding S.S.C.P.'s for Same Density, $T = 750$ eV.</td>
<td>115</td>
</tr>
<tr>
<td>3c.</td>
<td>The Effective Potential in $r$-space Compared to Corresponding S.S.C.P.'s for Three Different Densities, $T = 100$ eV.</td>
<td>116</td>
</tr>
<tr>
<td>4.</td>
<td>Neon Spectrum at Two Different Plasma Temperatures as a Function of Density.</td>
<td>117</td>
</tr>
<tr>
<td>5.</td>
<td>Neon Lyman-$\alpha$ Line Shifts Obtained Using the Effective Screened Potential Compared to Skupsky's Self-Consistent Calculations.</td>
<td>118</td>
</tr>
<tr>
<td>6.</td>
<td>Variation of the 'Universal' Curves as Functions of $t$: Exchange Energy and Exchange Potential Scaled by the Respective Zero Temperature Value.</td>
<td>119</td>
</tr>
<tr>
<td>Figure</td>
<td>Page</td>
<td></td>
</tr>
<tr>
<td>--------</td>
<td>------</td>
<td></td>
</tr>
<tr>
<td>7.</td>
<td>120</td>
<td></td>
</tr>
<tr>
<td>The Correlation Energy and the Exchange Energy as a Function of $t$ for Three Different Densities.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8.</td>
<td>121</td>
<td></td>
</tr>
<tr>
<td>The Exchange-Correlation Energy Along with the Corresponding Exchange Contribution as a Function of $t$.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>9.</td>
<td>122</td>
<td></td>
</tr>
<tr>
<td>The Correlation Potential and the Corresponding Exchange Potential as a Function of $t$ for Three Different Densities.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.</td>
<td>123</td>
<td></td>
</tr>
<tr>
<td>The Exchange-Correlation Potential Along with the Corresponding Exchange Contribution as a Function of $t$ for Two Densities.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>11.</td>
<td>124</td>
<td></td>
</tr>
<tr>
<td>The Exchange-Correlation Potential Scaled by the Respective Zero Temperature Value as a Function of Density at Three Different Temperatures.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>12.</td>
<td>125</td>
<td></td>
</tr>
<tr>
<td>The Cross-Over Temperature as a Function of Electron Density.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>13.</td>
<td>126</td>
<td></td>
</tr>
<tr>
<td>The Self-Consistent Hartree Potential with the Corresponding Charge Density Profile for a Neon Impurity in a Dense, Hot Plasma and the Corresponding Effective Kohn-Sham Potential.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
ABSTRACT

The generalization of the zero temperature local density functional theory of inhomogeneous electron systems to finite temperature ensembles is discussed. A local exchange-correlation potential, $V_{xc}$, needed for a finite temperature Kohn-Sham scheme, is developed based on the investigation of first-order exchange and 'ring'-diagram contribution to correlation effects for a wide range of electron densities and temperature. Comparison is made with existing results in the fully degenerate and non-degenerate limits. In the intermediate degeneracy region, the correlation effect is found to be enhanced—the importance of this for various physical systems is pointed out. An application of $V_{xc}$ is made to illustrate the effect on Kohn-Sham eigenvalues for a neon impurity embedded in a dense, laser plasma, and compared with corresponding self-consistent Hartree results. A fully self-consistent calculation of Perrot using our $V_{xc}$ for a proton in an electron gas is also discussed.

A connection is made between the finite temperature Kohn-Sham effective potential with the temperature dependent Lindhard screened potential. This gives a scheme to investigate the electron screening effects in the intermediate degeneracy region and interpolates
between the well-known Thomas-Fermi screening in the degenerate limit and Debye-screening in the classical limit. Applications are made to study the screened energy levels for charged impurities in dense, hot laser plasmas and in highly doped semiconductors. An estimate of Mott transition is also obtained. Results are compared with other screening models. The significance for plasma diagnostics of the striking differences obtained in the results is pointed out.
CHAPTER 1

INTRODUCTION

The study of the electronic properties of matter requires the investigation of interacting inhomogeneous system of electrons. This is a complicated quantum statistical problem. Because of the extreme complexity of the problem, many different schemes for approximate calculations have been developed over many years and the search for new ones continue. A practical and useful scheme developed over the last 15 years and the one that concerns us here is the local density functional theory of Kohn and Sham.\textsuperscript{1} In contrast to the quantum statistical methods, the electron density of the system is treated as a basic variable in this theory. The scheme has been very successfully applied to investigate the ground-state (zero temperature) electronic properties of physical systems—e.g., atoms, molecules, and solids. For an extensive review of such applications, one may refer to the article by Rajagopal.\textsuperscript{2}

The success of the zero temperature local density functional theory as a practical scheme encourages one to generalize the Kohn-Sham formalism to finite temperatures. This extension, only formally outlined by Mermin\textsuperscript{3}, would then enable one to study the electronic properties of physical systems in thermal equilibrium at finite temperatures. A practical and systematic development in this
direction has been lacking so far. The present work attempts to contribute in this important area.

A finite temperature theory requires the introduction of the equilibrium temperature $T$ as a variable, in addition to the electron density $n$. Depending on the physical situation, the effects of temperature could be very significant. A relevant temperature scale, in this context, is the Fermi temperature $T_F$, associated with a system of electrons of uniform density, $n$, defined as:

$$k_B T_F = \frac{\hbar^2}{2m} \left( \frac{3\pi^2 n}{3} \right)^{2/3}. \quad (1)$$

($k_B$ = Boltzmann constant, $\hbar$ = Planck constant, $m$ = electronic mass). The system of electrons behave as a highly degenerate, quantum system if the ratio $t = T/T_F$, is much less than unity. On the other hand, if $t \gg 1$, one has a classical, non-degenerate system. As we shall see later on, in the 'intermediate degeneracy' region ($t \approx 1$), the electronic properties exhibit interesting deviations from either the fully classical or fully quantum-mechanical behavior.

Depending on the physical system, the electronic density and temperature, of course, can vary widely. Our interest is primarily in situations where systems are in the 'intermediate degeneracy' range. Dense, hot laser-imploded plasmas, shock compressed solids raised to elevated temperatures, highly doped semiconductors at room
temperature, astrophysical plasmas in exotic conditions (interior of a white dwarf, for example) are among a wide class of physical systems that fall in this category. A comparison of Tables 1(a) and 1(b) illustrates this.

A finite temperature Kohn-Sham theory, besides being a general scheme, is particularly useful for application to the type of systems mentioned above. This is a major motivation for the present work.

Let us first review the basic aspects of the zero temperature formalism before considering the finite temperature generalization of the Kohn-Sham scheme. The formalism rests on the following theorem due to Hohenberg and Kohn $^4$: For an interacting system of electrons in the presence of a static external potential $\mathbf{v}(\mathbf{r})$, there exists a universal functional $F[n(\mathbf{r})]$ of the electron density $n(\mathbf{r})$ independent of $\mathbf{v}(\mathbf{r})$, such that the expression

$$ E \equiv \int \mathbf{v}(\mathbf{r}) \ n(\mathbf{r}) \ d\mathbf{r} + F[n(\mathbf{r})] $$

has as its minimum value, the correct ground-state energy of the electron-system associated with $\mathbf{v}(\mathbf{r})$ and the corresponding $n(\mathbf{r})$ is the correct ground-state density in presence of $\mathbf{v}(\mathbf{r})$.

Further, separating out the electrostatic Coulomb interaction term from $F[n]$,
\[ P[n(\vec{r})] = \frac{e^2}{2} \int \frac{n(\vec{r}) n(\vec{r}')}{|\vec{r} - \vec{r}'|} \, d\vec{r} \, d\vec{r}' + G[n(\vec{r})], \quad (3) \]

with

\[ G[n(\vec{r})] = T_s[n(\vec{r})] + E_{\text{XC}}[n(\vec{r})], \quad (4) \]

where \( T_s[n] \) is the kinetic energy of a system of non-interacting electrons with density \( n(\vec{r}) \) and \( E_{\text{XC}}[n] \) is the exchange-correlation energy functional of the interacting electrons with density \( n(\vec{r}) \), they showed that \( G[n(\vec{r})] \) is a universal functional of the density.

From the stationary property of Eq. (1), subject to the condition that the total number of particles,

\[ \int n(\vec{r}) \, d\vec{r} = N \quad (5) \]

is fixed, one obtains

\[
\begin{align*}
\int d\vec{r} \, \delta n(\vec{r}) \left[ \frac{\delta T_s[n]}{\delta n(r)} + v(\vec{r}) \right. \\
+ \frac{e^2}{2} \int \frac{n(\vec{r}')}{|\vec{r} - \vec{r}'|} \, d\vec{r}' + \frac{\delta E_{\text{XC}}[n]}{\delta n(r)} \left. \right] = 0 \quad (6)
\end{align*}
\]

As argued by Kohn and Sham, Eq. (5) and (6) physically implies the equation of motion of a system of non-interacting electrons moving in an effective one-particle potential.
\[ V_{\text{eff}}(\mathbf{r}, n(\mathbf{r})) = v(\mathbf{r}) + e^2 \int \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' + V_{\text{xc}}[n(\mathbf{r})] \]  

where

\[ V_{\text{xc}}[n(\mathbf{r})] = \frac{\delta E_{\text{xc}}[n(\mathbf{r})]}{\delta n(\mathbf{r})} \]  

is defined to be the exchange-correlation-potential, also a functional of density.

Therefore, one has, effectively, a set of single-particle Schrödinger-like equations to be solved self-consistently:

\[ \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{eff}}(\mathbf{r}, n(\mathbf{r})) \right] \psi_i(\mathbf{r}) = \epsilon_i \psi_i(\mathbf{r}) \]  

with

\[ V_{\text{eff}}(\mathbf{r}, n(\mathbf{r})) = v(\mathbf{r}) + e^2 \int \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' + V_{\text{xc}}[n(\mathbf{r})], \]  

and the particle-density \( n(\mathbf{r}) \) is given by

\[ n(\mathbf{r}) = \frac{N}{\sum_{i=1}^{N} |\psi_i(\mathbf{r})|^2} \]  

where \( N \) is the total number of electrons.

Thus the many-body problem has been reduced to an effective one-body problem. For a given \( V_{\text{eff}} \), one obtains the density \( n(\mathbf{r}) \) from (9c) by solving the effective Schrödinger eq. (9a), and iterate until self-consistency is achieved. The identification of \( \delta T_S/\delta n(\mathbf{r}) \) by the kinetic energy operator \( (-\hbar^2 \nabla^2/2m) \) is a subtle step in
the reduction to one-body problem. This simplicity underlines the extensive use of this scheme for practical calculations.

The total ground-state energy is then given by

\[ E = \sum_{i=1}^{N} \epsilon_i - \frac{e^2}{2} \int \int \frac{n(\mathbf{r}) n(\mathbf{r'})}{|\mathbf{r} - \mathbf{r'}|} d\mathbf{r} d\mathbf{r'} + E_{xc}[n(r)] \]

\[ - \int n(\mathbf{r}) v_{xc}[n(\mathbf{r})] d\mathbf{r} \]  

(10)

and

\[ T_s[n(\mathbf{r})] = \sum_{i=1}^{N} \epsilon_i - \int n(\mathbf{r}) v_{eff}(n(\mathbf{r})) d\mathbf{r}. \]  

(11)

Up to this point, the theory is exact; the universal functional \( E_{xc}[n] \) is unknown and no clear scheme for constructing it is outlined. One of the popular and developed schemes is the local density approximation (LDF), here one assumes that the exchange-correlation energy functional could be represented as

\[ E_{xc}[n(r)] = \int n(\mathbf{r}) \varepsilon_{xc}(n(\mathbf{r})) d\mathbf{r} \]  

(12)

with \( \varepsilon_{xc}(n) \) as the exchange-correlation energy per electron of an interacting uniform gas of density \( n \). Then

\[ v_{xc}[n(r)] = \frac{\delta E_{xc}}{\delta n(r)} = \frac{d}{dn} (n \varepsilon_{xc}) = \nu_{xc} \]  

(13)

and total energy
\[ E = \sum_i \varepsilon_i - \frac{e^2}{2} \iint n(\vec{r}) \frac{\partial^2}{(\vec{r} - \vec{r}')^2} \, d\vec{r} \, d\vec{r}' \]

\[ + \int n(\vec{r}) \left[ \varepsilon_{xc}(n(\vec{r})) - u_{xc}(n(r)) \right] \]  

(14)

The LDF-scheme then is based on the validity of the assumption (12). This is expected to be adequate for slowly varying density. As shown by Kohn and Sham, the results of this procedure are exact in the limit of (i) high density and for (ii) slowly varying density. The practical advantage of the LDF-scheme is that it is like the familiar Hartree scheme, in contrast to the much more complicated non-local density functional scheme, accounts for its extensive use in a variety of calculations. The other crucial advantage is that \( \varepsilon_{xc} \) is obtained from the existing theories of uniform electron gas.

Finite Temperature Generalization:

Let us now consider the generalization of the zero temperature scheme to finite temperatures. An important step in this direction was taken by Mermin by generalizing the Hohenberg-Kohn theorem to non-zero temperatures. He showed that (i) In the grand canonical ensemble at a given temperature \( T \) and chemical potential \( \mu \), the equilibrium density \( n(\vec{r}) \) of an inhomogeneous electron-system in a static external potential \( v(\vec{r}) \) is uniquely determined by

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
\( v(\mathbf{r}) \), (ii) the correct equilibrium density \( n(\mathbf{r}) \), for a given \( v(\mathbf{r}) \) minimizes the grand potential \( \Omega[n(\mathbf{r}),T] \). (The theorem is valid for canonical ensemble also). Further, \( \Omega \) could be written as

\[
\Omega = \int v(\mathbf{r}) \, n(\mathbf{r}) \, d\mathbf{r} + \frac{e^2}{2} \int \int n(\mathbf{r}) n(\mathbf{r'}) \, d\mathbf{r} \, d\mathbf{r'} \, |\mathbf{r} - \mathbf{r'}|^{-1}
\]

\[ + G[n(\mathbf{r})] - \mu \int n(\mathbf{r}) \, d\mathbf{r} \]  

(15)

where \( G[n] \) is a unique functional of density:

\[
G[n] = G_s[n] + F_{xc}[n] ;
\]

(16a)

here

\[
G_s[n] = T_s[n] - T S_s[n]
\]

(16b)

where \( T_s[n] \) and \( S_s[n] \) are, respectively, the kinetic energy and entropy of non-interacting electrons with density \( n(\mathbf{r}) \) at temperature \( T \); and \( F_{xc}[n] \) is the exchange and correlation contribution to the free exchange.

Let us note that unlike the zero temperature formalism, the particle density \( n(\mathbf{r}) \) and consequently other quantities \( \Omega \) or \( F_{xc} \) etc., now depends on temperature \( T \). (The explicit \( T \)-dependence of \( n(\mathbf{r}) \) will be given presently). Also, all physical quantities are now given by their ensemble averages, unlike the \( T = 0 \) formalism where only expectation values of appropriate operators were needed. Again, \( F_{xc} \) is unknown.
In the local approximation,

$$F_{xc}[n] = \int \Omega_{xc}[n(\mathbf{r})] \, d\mathbf{r}$$  \hspace{1cm} (17)

where $\Omega_{xc}[n]$ is the exchange-correlation energy density appropriate to an interacting uniform electron-gas of density $n$ in thermal equilibrium at temperature $T$. Analogous to zero-temperature case, the minimal property of $\Omega$ as given by (15) leads to the following system of single-particle equation to be solved self consistently:

$$\left\{ \begin{array}{l}
\frac{-\hbar^2}{2m} \nabla^2 + V_{\text{eff}}[\mathbf{r},n(\mathbf{r}),T] \psi_i(\mathbf{r}) = \epsilon_i \psi_i(\mathbf{r}) \, , \\
\end{array} \right. \hspace{1cm} (18a)$$

$$V_{\text{eff}}[\mathbf{r},n(\mathbf{r}),T] = v(\mathbf{r}) + e^2 \int \frac{n(\mathbf{r}',T) \, d\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|}$$

$$+ V_{xc}[n(\mathbf{r}),T] \hspace{1cm} (18b)$$

and

$$n(\mathbf{r},T) = \frac{N}{\sum_{i=1}^{\infty} |\psi_i(\mathbf{r})|^2 \left[ e^{\beta(\epsilon_i - \mu)} \right] + 1} \hspace{1cm} (18c)$$

Here, $V_{xc}[n(\mathbf{r}),T] = \frac{\delta \Omega_{xc}[n(\mathbf{r}),T]}{\delta n(\mathbf{r})}$ is the exchange-correlation potential. ($\beta \equiv 1/(k_B T)$, $k_B$ = Boltzmann constant).

The chemical potential $\mu$ is determined by

$$N = \int n(\mathbf{r},T) \, d\mathbf{r} = \sum_i \frac{1}{e^{\beta(\epsilon_i - \mu)} + 1} = \sum_i f_i$$  \hspace{1cm} (18d)

where the sum is over all occupied states, both bound and
The grand potential $\Omega[n,T]$ is given by

$$\Omega = \sum_i \varepsilon_i f_i - \frac{e^2}{2} \iint \frac{n(\mathbf{r},T) n(\mathbf{r}',T) \, d\mathbf{r} \, d\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|}$$

$$+ \Omega_{XC}[n(\mathbf{r}),T] - \int n(\mathbf{r},T) V_{XC}(n(\mathbf{r}),T) \, d\mathbf{r} \quad (18e)$$

Equations (18a)-(18d) constitutes the basic system of equations representing the formal generalization of the Kohn-Sham scheme to finite temperatures. In the rest of this work, we will be concerned with various aspects of the scheme, as well as its actual application.

As mentioned previously, the reduction of a complicated many-body problem to an effective one-body problem is the first appealing feature of the scheme. The finite temperature generalization removes the zero-temperature restriction which, of course, is an idealization and allows one to examine the excited equilibrium states of the system as well. Being so general in formulation, the scheme could, in principle, be applied to study static properties of a wide variety of physical systems in thermal equilibrium.

In the subsequent chapters, we shall present results of our investigation of some problems related to dense, hot plasmas and semiconductors at room temperatures.

For studying properties of matter in thermal equilibrium, an alternative scheme, namely the Thomas-Fermi
method\textsuperscript{5} (TF), has been in existence since the 1920's. In its original form, all exchange-correlation effects are neglected, unlike the density functional formalism. This, of course, is a poor approximation in most cases, and we will discuss it in detail later on. In fact, in many interesting cases, these many-body effects are known to play a crucial role—the surface properties of solids, for instance. In the Thomas-Fermi-Dirac (TFD) method\textsuperscript{6}, the exchange-effect is included via a local potential of the form $-\alpha n^{1/3}(r)$ with $\alpha$ an adjustable constant.

This naturally gives improved results over the TF-scheme. However, correlation is still not accounted for, and as we shall see in detail later on from our investigations, the appropriate temperature-dependence of exchange effect brings out the inadequacy of the $-\alpha n^{1/3}(r)$ form.

Secondly, in the TF-method, the kinetic energy density term is approximated in the $n^{2/3}$-form, appropriate to the ease of slowly varying density only. On the other hand, in the density-functional scheme, kinetic energy term is treated exactly. This clearly is very important and naturally leads to better results. Also, as pointed out by Kohn and Sham\textsuperscript{1}, the LDF-scheme does not lead to an infinite density near an atomic nucleus, unlike the TF-method. In addition, it automatically reproduces the quantum density oscillations, such as the density fluctuations due to atomic shell structures. The TF-method or other refinements of it do not give this. However, a
recent Thomas-Fermi-shell model\textsuperscript{7} introduces the shell structure by incorporating the bound and resonance state contribution separately to the total electronic density. This is an artificial method in comparison to the density functional one where this feature comes out in a natural way.

In spite of its shortcomings, the TF-method and its improvements have provided useful results for studying properties of matter in thermal equilibrium. However, from the above comparison, it is clear that a finite temperature LDF-scheme is a superior one and thus is expected to lead to better results. This is a major motivation for the present work.

A crucial ingredient in a systematic development of the finite temperature scheme is the appropriate exchange-correlation potential $V_{xc}[n,T]$, which has been lacking so far. McMahan and Ross\textsuperscript{8} study the high temperature electron-band structures to understand shock compression data using a zero temperature local $V_{xc}$. Rozanyai\textsuperscript{7} examines atomic properties at high temperatures and pressures and uses a local potential which interpolates approximately between the high density, low temperature and the low density, high temperature forms. Recently, Liberman\textsuperscript{10} proposed a model for condensed matter at arbitrary temperatures. While the model itself is probably the best one
of its kind, he also employs the zero-temperature Kohn-Sham or Hedin-Lundquist potential. Let us quote here that in the work of Ref. 8 and 10, the temperature dependence is brought in only through the expression for local density, Eq. (18c). However, there is an explicit additional temperature dependence of $V_{xc}(n,T)$ arising from that of $\Omega_{xc}(n,T)$ which we will show is very important.

This dissertation is organized as follows: In chapter II, we point out the connection between the Kohn-Sham effective potential with the screened effective potential. The screening of an impurity charge embedded in a plasma is treated by using the R.P.A. dielectric function generalized to finite temperatures. This gives us a screening model that interpolates naturally between the Debye and the Thomas-Fermi screening. Application is made to study the energy level and line shifts of a singly charged impurity as well as a neon impurity in a hot, dense laser produced plasmas. In the intermediate degeneracy region, the results are compared to Debye and Thomas-Fermi results as well as to a self-consistent calculation by Skupsky. Implications of these results to plasma diagnostics are pointed out.

Another application of our scheme is made to study the screened shallow impurity states in a doped semiconductor at room temperature. The criterion for Mott
transition is also discussed.

In chapter III, the first-order exchange effects for electron-systems at finite temperatures is investigated. The Kohn-Sham local exchange potential is generalized to non-zero temperatures. Aspects of 'universality' in this scheme is discussed.

The electron correlation effects at finite temperatures are investigated in chapter IV using the sum of 'ring' diagrams as an approximation. The relative importance of correlation effects compared to exchange effects is examined. The exchange-correlation energies $\Omega_{xc}$ and potentials $V_{xc}$ are computed for a wide range of electron densities and temperatures.

In chapter V, we discuss an application of $V_{xc}$ to illustrate its effect on the Kohn-Sham eigenvalues for a neon impurity in a hot, dense laser-produced plasma. Comparison is made with a self-consistant Hartree calculation of Liberman (private communication). A full self-consistent calculation by Perrot\textsuperscript{12}, using our $V_{xc}$, is also discussed.

The general conclusions are summarized in chapter VI.
CHAPTER II

ELECTRON SCREENING EFFECTS AT FINITE TEMPERATURES

In this chapter, we will discuss an important many-body problem--the electron screening effect of a static impurity charge $+Ze$ embedded in a plasma of density, $n$, in thermal equilibrium at a temperature, $T$. The basic questions we are concerned with here are the following: (i) What is the effective potential $V_{\text{eff}}(\hat{r})$ due to the impurity charge $+Ze$ as modified by the polarisation of the surrounding electron-gas and (ii) the screening shifts of the bound-state energy levels of the "hydrogen-like" states supported by this $V_{\text{eff}}(\hat{r})$, as functions of $n$ and $T$.

This problem of screening is of central importance in many different areas of physics. In astrophysics, the disappearance of spectral lines near the series limit has long been observed and attributed to screening affects. In plasma physics, this is important both for (i) diagnostic studies--here, the intensities and line profiles due to electronic transitions between shifted energy levels of ionic impurities are used to determine plasma densities and temperatures, and for (ii) thermodynamic properties: the interacting part of the partition function, for example, requires a knowledge of the shifted energy levels. The calculation of 'rate coefficients', similarly, requires...
both the number and the energies of these shifted levels. The screening due to mobile charge carriers is important in semiconductors also—particularly for a discussion of the optical properties and the Mott transition.

Traditionally, static screened coulomb potentials (SSCP) have been used to describe these screening effects. In high temperature plasmas, Debye-screened potential

$$V_D(r,n,T) = -\frac{Ze^2}{r} e^{-r\zeta_D}$$ (19)

where $\zeta_D = (4\pi ne^2/k_B T)^{1/2}$ is the Debye screening length ($e =$ electronic charge, $k_B =$ Boltzmann constant) has been used extensively. In semiconductors, on the other hand, Thomas-Fermi screened potential

$$V_{TF}(r,n) = -\frac{Ze^2}{r} e^{-r\zeta_{TF}}$$ (20)

with $\zeta_{TF} = (4k_F^2/\pi a_o)^{1/2}$ ($a_o =$ Bohr radius, $k_F =$ (3$\pi^2 n)^{1/3}$ is the Fermi rarevector) is often employed. The region of validity of these models will be examined quantitatively in subsequent sections. The effective impurity potential, $V_{\text{eff}}(r,n,T)$, we present below goes over to the Debye and the TF-potentials in appropriate limits and reveals the fact that there exist important regions of plasma-densities and temperatures where neither of the models (19) nor (20) is adequate.
I. The Effective Screened Potential

The effective impurity potential we will be dealing with could be derived in different ways. Here, we present the derivation that brings out its connection with the density functional scheme in a clear fashion.

Let us recall the effective potential, eq. (18b) obtained in the temperature-dependent Kohn-Sham scheme. The external potential, in this case, is simply the Coulomb potential due to the static impurity charge $+Ze$ embedded in the plasma. Therefore,

$$V(r) = -\frac{Ze^2}{r}.$$ 

Now, if one neglects the exchange-correlation effects completely, by setting $V_{xc} = 0$, (we will examine the validity of this approximation in detail in the following chapters) we have,

$$V_{\text{eff}}[\mathbf{r}, n, T] = -\frac{Ze^2}{r} + e^2 \int \frac{n(\mathbf{r'}, T) \, d\mathbf{r'}}{|\mathbf{r} - \mathbf{r'}|}$$  

(21)

Physically, the external impurity charge $+Ze$ polarises the medium and brings about a redistribution of the electronic charge density, $n(\mathbf{r}, T)$ around it.

Going over to momentum space, and using the convolution theorem, we have,

$$V_{\text{eff}}(q) = -\frac{4\pi Ze^2}{q^2} + \frac{4\pi e^2}{q^2} n(q, T)$$  

(22)
where \( q \) is the momentum variable. If the density deviation is approximated as responding linearly to the effective potential via an appropriate response function, \( \chi(q,n,T) \),

\[
n(q,T) = \chi(q,n,T) \, V_{\text{eff}}(q)
\]

Then, we obtain,

\[
V_{\text{eff}}(q) = -\frac{4\pi e^2}{q^2} \frac{1}{1 - \left(\frac{4\pi e^2}{q^2}\right) \chi(q,n,T)}.
\]

The function \( \chi(q) \) is really the retarded part of the time-ordered density correlation function and is complex in general. Physically, it represents how the density deviation at two different spatial regions in a medium are correlated. At zero temperature, one has available, the Random Phase Approximation (R.P.A.) result for \( \chi(q) \) due to Lindhard\(^{13}\). In this approximation, the static \( \chi(q,\omega=0) \) is purely real.

Since we are interested in temperature-dependent properties, we use the Lindhard function generalized to non-zero temperatures for \( \chi(q,n,T) \).

\[
\chi(q,n,T) = -2 \int \frac{d^3 p}{(2\pi)^3} \frac{f(p+q) - f(p)}{(\epsilon_p + \epsilon_{p+q})}\]

with \( \epsilon_p = \hbar^2 p^2 / 2m \), and \( f(p) \) is the Fermi function for the electrons:
$$f(p) = \frac{1}{e^{\frac{\beta (e_p - \mu)}{k_B T}} + 1}$$  (26)

$$(\beta = 1/k_B T)$$. The chemical potential $\mu$ is to be determined from the phase-space integral

$$n = 2 \int \frac{d^3 k}{(2\pi)^3} \frac{1}{e^{\beta (\frac{\mu^2 k^2}{2m} - \mu)} + 1}$$  (27)

On carrying out the angular integration, it is easy to express $\chi(q,n,T)$ as a one-dimensional integral:

$$\frac{4\pi e^2}{q^2} \chi(q,n,T) = -\left(\frac{4k_F}{\pi a_0}\right) \frac{1}{q^3} \int^\infty_0 dk f(k) \ln \frac{|q+2k|}{q-2k}$$  (28)

Using (28) for $\chi(q,n,T)$; the effective impurity potential we obtain is

$$V_{\text{eff}}(r,n,T) = -\frac{2e^2}{\pi} \int dq \left(\frac{\sin qr}{qr}\right) \frac{1}{q^2} \frac{4\pi e^2}{q^2} \frac{1}{\chi(q,n,T)}$$  (29)

For subsequent analysis as also for computational purposes, it is convenient to introduce the dimensionless temperature variable $t = T/T_F$, where $T_F$ is the fermi temperature defined via eq. (1). Also, we measure all momenta in units of fermi momentum $k_F = \left(3\pi^2 n\right)^{1/3}$.
One immediate consequence is that eq. (27) could be recast in the form:

\[
\frac{1}{3} = \int_0^\infty dx \frac{x^2}{\exp[t^{-1}x^2-\alpha]+1} ,
\]

with \( \alpha = \beta \mu \). This shows that the degeneracy parameter \( \alpha \) is a function of \( t \)-only; and does not depend on \( n \) and \( T \) separately. Different sets of densities and temperatures, corresponding to the same \( t \)-value would involve the same value of \( \alpha \). This, in turn, gives rise to the feature of 'universality' in various physical quantities as we shall see presently.

In terms of these scaled variables, we have

\[
V_{\text{eff}}(r,n,t) = -\frac{2e^2}{\pi} k_F \int_0^\infty dQ \frac{\sin(Qk_Fr)}{(Qk_F)^2} \frac{1}{1+\zeta^2 [Q,n,t]/Q^2}
\]

where the effective screening parameter \( \zeta \) is given by

\[
\zeta^2(Q,n,T) = \frac{4}{\pi a_Q k_F Q} \int_0^\infty dx \frac{x}{1 + \exp[t^{-1}x^2-\alpha]} \ln \frac{x+Q/2}{x-Q/2} .
\]
(1) The effective screening parameter $\zeta$ is momentum dependent in contrast to $\zeta_{TF}$ or $\zeta_D$. The density and temperature (or t-) dependence enters both via the prefactor is also through the Fermi function. This is reflected in the effective screened potential $V_{\text{eff}}(r,n,t)$ as well.

(2) In the limit of small momentum transfer, $Q \to 0$, one obtains

$$\zeta^2(Q,n,t) \to \frac{4}{\pi a_0 k_F} \int_0^\infty dx \frac{1}{\exp[t^{-1}x^2 - \alpha] + 1}$$

which is independent of $Q$. Thus,

$$\zeta^2(Q = 0,n,t)/\zeta^2_{TF},$$

a universal function of t-only:

$$\frac{\zeta^2(Q=0,n,t)}{\zeta^2_{TF}} = \int_0^\infty dx f(x). \quad (33)$$

In this $Q \to 0$ limit, our $V_{\text{eff}}(r)$ goes over to the SSCP-form;

$$V_{\text{eff}}(r,n,t) \to V_{\zeta}(r) = -\frac{ze^2}{r} e^{-rk_F^2 \zeta(n,t)} \quad (34)$$

(3) Further, as $t \to \infty$ (non-degenerate, classical limit).

$$\frac{\mu}{\varepsilon_F} = at + t \ln \left( \frac{4}{3} \pi^{-1/2} \zeta^{-3/2} \right) + \ldots \quad (35)$$
and

\[ \frac{\zeta^2(n,t)}{\zeta_{TF}^2} \rightarrow \frac{2}{3t} = \frac{\zeta_D^2}{\zeta_{TF}^2}. \]  

(36)

Correspondingly, the effective potential approaches the Debye-screened potential in this limit:

\[ V_{\text{eff}}(r,n,t) \rightarrow V_D(r) = -\frac{2e^2}{r} e^{-r/k_F \zeta_D}. \]  

(37)

In the opposite limit of \( t \rightarrow 0 \) (fully degenerate, quantum limit), we have

\[ \frac{\mu}{\zeta_F} + 1 - \frac{\pi^2}{12} t^2 + \ldots \ldots \]  

(38)

and

\[ \frac{\zeta^2(n,t)}{\zeta_{TF}^2} \rightarrow 1 - \frac{\pi^2}{12} t^2 - \frac{191\pi^4}{5760} t^4 + \ldots. \]  

(39)

Thus, one recovers the Thomas-Fermi screened potential

\[ V_{\text{eff}}(r,n,t) \rightarrow V_{\text{TF}}(r) = -\frac{2e^2}{r} e^{-r/k_F \zeta_{TF}}. \]  

(40)

The above analysis brings out several important features of our effective screened potential \( V_{\text{eff}}(r,n,t) \). At large distances from the impurity, the screening is essentially Yukawa-like, eq. (34), however, the screening parameter \( \zeta[Q=0,n,t] \) could, in general, be very different from
either Debye or TF-form. $Q \to 0$ approximation is better in the high-density limit, as we shall see more fully later on. In general, the full momentum dependence makes the screening significantly different from any SSCP-forms that are frequently used.

The asymptotic forms for $\zeta^2(Q=0,n,t)$ could this be used to establish quantitatively the 'region intermediate degeneracy' where neither Debye nor Thomas-Fermi screening is really valid. Curve (a) of Fig. 1 shows a 'universal' plot of $\zeta^2(Q=0,n,t)/\zeta_{TP}^2$ as a function of $t$ obtained numerically from eq. (33) along with eq. (30). This shows that in the domain $0.2 < t < 3.5$, the screening parameter differs from the TF or Debye-values by 6% or more. Numerical values of $\zeta^2(Q=0,n,t)/\zeta_{TP}^2$ for different values of $t$ are listed in Table 1.

It should be noted that the region of intermediate degeneracy one could obtain by examining the departure from asymptotic form of $\mu/E_F$ as a function of $t$ (curve (b), Fig. 1) is slightly different: $0.3 < t < 2.5$. For the discussion of screening effect, the relevant range of $t$ should be obtained from the behaviour of $\zeta(Q=0,n,t)$.

Let us note here that this range of $t$-values includes a wide range of interesting plasma densities and temperatures. For example, for a laser-fusion plasma of $n \sim 10^{24}$ electrons/cm$^2$, $T \sim 10^6$ K, $t \sim 2.6$ and is thus included in
this region. The usefulness of this 'universal' curve is that for any given electron density and temperature, one can obtain the appropriate screening parameter $\zeta[n,t]$ readily from this curve.

The parameter $\zeta[n,t]$ contains the correct degeneracy effect. The full $Q$-dependence of $\zeta^2(Q,n,t)$ which is missed by SSCP's, also plays a significant role. For illustration, we have plotted $V_{\text{eff}}(Q,n,t) = -\frac{4\pi Ze^2}{k_F^2}$ versus $Q$ (full curve) in Fig. 2 for a representative set of plasma parameters: $n \approx 6.8 \times 10^{21}$ electrons cm$^{-3}$ and $T \approx 10^4$ K ($t \approx 0.66$). For comparison, $V_{\zeta}(Q) = -\frac{4\pi Ze^2}{k_F^2} \frac{1}{Q^2 + \zeta^2(Q=0,n,t)}$ (chain curve) and $V_D(Q) = -\frac{4\pi Ze^2}{k_F^2} \frac{1}{Q^2 + \zeta_D^2}$ (broken curve) for the same $n$ and $T$-values are also plotted. The plot shows that (i) the full effective potential is significantly deeper than the corresponding $V_D(Q)$ and $V_{\zeta}(Q)$ over a large range of $Q$ (note the log-scale). Consequently, this should affect the bound electronic states supported by $V_{\text{eff}}$, as we shall see shortly. (ii) For small $Q$-values ($Q \approx 0.2$), $V_{\text{eff}}(Q)$ differs from $V_D(Q)$ by about 48% and all of it is due to $t$-dependence. (iii) In the intermediate $Q$-range,
For $1 \leq Q \leq 10$, $V_{\text{eff}}(Q)$ differs from $V_D(Q)$ as well as $V_c(Q)$ by 8% to 25% due to the fact that the correct $Q$-dependence is missed in the SSCP-approximation. (iv) For large $Q$, all the potentials merge with each other as they should, since very near the impurity charge $(r=0)$, the potential is essentially the bare Coulomb potential. The behavior of $V_{\text{eff}}$ as a function of $\mathbf{r}$ will be examined later on.

(4) A pleasant feature of this scheme is that $V_{\text{eff}}$ satisfies the consistency condition that the total induced charge density brought about by the polarization effect exactly compensates the external charge $\pm e$ introduced into the plasma:

$$-e \int d^3r \, \delta n_{\text{ind}}(r) = -Ze. \quad (41)$$

This is readily seen as follows:

$$-e \int \delta n_{\text{ind}}(r) \, d^3r = -e \int d^3r \int \frac{d^3q}{(2\pi)^3} \, e^{i\mathbf{q}\cdot\mathbf{r}} \, \delta n_{\text{ind}}(q)$$

$$= -e \int d^3r \int \frac{d^3q}{(2\pi)^3} \, e^{i\mathbf{q}\cdot\mathbf{r}} \, \chi(q) \, V_{\text{eff}}(q) \quad \text{using (23)}$$

$$= -Ze \int d^3r \int \frac{d^3q}{(2\pi)^3} \, e^{i\mathbf{q}\cdot\mathbf{r}} \left[ -\frac{4\pi e^2 \chi(q)}{q^2 - 4\pi e^2 \chi(q)} \right], \quad \text{using (24)}$$
Thus, the screening is complete over large distances.

Also, note that the induced charge density $\delta n_{\text{ind}}(r)$ is finite everywhere, including the origin.

II. Ground State Energy—A Variational Calculation

As a first application of the effective screened potential, we now compute, by the variational method, the ground state energy $E$ of an electron bound by the attractive impurity potential with $Z = 1$. The purpose is to study the screening effect in the intermediate degeneracy region on the electron binding energy using our scheme and to compare with corresponding results obtained by using $V_D(r)$ and $V_\phi(r)$. An analogous study has been made by Krieger and Nightingale in connection to Mott transition in a semiconductor at zero temperature. This is a finite temperature generalisation of their work and applied to a dense, hot laser-produced plasma.

Choosing the normalized hydrogenic trial solution

$$\psi_B(r) = \left(\frac{\beta^3}{\pi}\right)^{1/2} e^{-\beta r},$$

where $\beta$ is a real positive parameter to be determined by minimizing the energy, the ground-state energy is given by
corresponds to $t$ of about 0.3. Thus, the temperature effect reduces the screening effect slightly, producing a deeper potential. However, the difference is quite small.

Thus, the critical density moves to a slightly higher value so that the screening is just sufficient to remove the last bound state.

The experimental result of Alexander and Holocomb\textsuperscript{25} seems to predict a substantially lower critical density $n_{c}^{1/3} \approx 0.22$. As pointed out by Greene\textsuperscript{25 et al.}, the hydrogenic trial function is not very adequate in this case. Their calculation using Hülthen trial function with appropriate valley degeneracy (4 for Silicon) improved the Mott criterion substantially: $n_{c}^{1/3} \approx 0.27$. Further calculation by Aldrich\textsuperscript{26} which includes the Silicon mass anistropy gives $n_{c}^{1/3} \approx 0.25$. Let us note here that a self-consistent LDA-calculation has also been performed by Rose, Shore, and Sander\textsuperscript{27} which predicts a metal-insulator transition at a much higher density ($n_{c} \approx 10^{22}$ cm$^{-3}$).

From the results presented so far, we see that useful estimates of the energy levels, line shifts etc. could be obtained using the temperature dependent Lindhard screened potential as a model impurity potential in dense, hot plasmas as well as semiconductor materials. The density and temperature dependence are included in this scheme in a natural way, in contrast to the Ion-sphere model. In the
\[ E_\varphi(\beta) = \left< \psi_\varphi \right| \frac{\hbar^2}{2m} \nabla^2 + V_{\text{eff}}(r,n,t) \left| \psi_\varphi \right> \]
\[
= \frac{\hbar^2 \beta^2}{2m} - \frac{e^2 \beta}{\pi} \int_0^\infty \frac{Q^4 \beta^4}{(Q^2 k_F^2 + 4\beta^2)^2} \frac{1}{[Q^2 + \zeta^2(Q,n,t)]^2} \]

with \( \zeta^2(Q,n,t) \) given by eq. (32).

To obtain (43), we used eq. (31) and performed the \( r \)-integration first. If one uses SSCP potentials of the form \( V_\zeta(r) = -\frac{e^2}{r} e^{-r\zeta[n,t]} \), then one has (using \( \psi_\alpha(r) = \left( \frac{\alpha^3}{\pi} \right)^{1/2} e^{-\alpha r} \)):

\[
E_\varphi(\alpha) = \frac{\hbar^2}{2m} \alpha^2 - \frac{e^2 \alpha^3}{(\alpha + \zeta/2)^2} \quad (44)
\]

The condition \( \frac{\partial E_\varphi(\alpha)}{\partial \alpha} = 0 \) leads to the cubic equation for \( \alpha \):

\[
\alpha^3 + \alpha^2 \left( \frac{3}{2} \frac{\zeta^2}{\alpha_0} - \frac{1}{\alpha_0} \right) + \alpha \left( \frac{3}{2} \frac{\zeta^2}{\alpha_0} - \frac{3}{2} \frac{\zeta^2}{\alpha_0} \right) + \frac{1}{8} \zeta^3 = 0. \quad (45)
\]

The correct root is chosen using the minimum condition,

\[
\frac{\partial^2 E_\varphi(\alpha)}{\partial \alpha^2} = e^2 \left( \frac{a_0}{a_0} - \frac{6a_0}{(a_0 + \zeta/2)^2} + \frac{12a_0^2}{(a_0 + \zeta/2)^3} - \frac{6a_0^3}{(a_0 + \zeta/2)^4} \right) > 0.
\quad (46)
\]

Computed values of \( E_\varphi \) by using \( V_{\text{eff}}, V_\zeta \) and \( V_D \) for a representative set of plasma densities and temperatures within the region of intermediate degeneracies are listed.
in Table 3. The differences in value of $E_o$ obtained from different models are quite striking. It clearly illustrates that the use of SSCP's in intermediate degeneracy region could lead to serious errors.

Physically, the large differences in computed values of $E_o$ could best be understood by referring to Fig. 2. Since the effective potential is deeper than the corresponding SSCP, the wavefunction is pulled in and hence the variational $\beta$ is always larger than $\alpha$. The consequent change in the form factor of the wavefunction

$$
\int e^{ik_F \cdot Q \cdot r} |\psi(\mathbf{r})|^2 \, d^3r \, \alpha \frac{Q^2 \beta^4}{(Q^2 k_F^2 + 4\beta^2)^2}
$$

is plotted in Fig. 2. For $V_{\text{eff}}$, the form factor is significantly larger than the corresponding quantity for $V_D$ in the range $2 < Q < 100$ (by about 17 times at $Q = 4$). Thus, in view of eq. (43), we see that for the small and intermediate $Q$-values, the major differences in $E_o$ come from the differences in the $V_{\text{eff}}(Q)$ from $V_{\text{SSCP}}(Q)$, whereas in large $Q$-range, although the potentials merge with each other, the large differences in form factors cause a further substantial change. A perturbation calculation misses this, since the changes in wave functions are not accounted for.
III. Bound State Spectrum due to $V_{\text{eff}}$: Neon impurity in dense, hot plasmas.

The sharp differences of ground-state energy values given by our $V_{\text{eff}}$ from the corresponding results obtained by using SSCP's, suggest that the effect on higher levels are likely to be even more pronounced. Since the energy levels are lower than the corresponding SSCP-values, the number of bound-states that the effective potential could support as well as the level separations are likely to be different. These have implications in a variety of plasma calculations. An accurate determination of the spectrum calls for solving the Schrödinger equation numerically with the effective screened impurity potential $V_{\text{eff}}(\vec{r}, n, t)$.

Numerical computation of $V_{\text{eff}}$ directly from eq. (31) turns out to be extremely difficult because of long-range oscillatory nature of the integrand and very slow convergence for large $Q$. This is circumvented by noting that

$$
\zeta^2(Q, n, t \alpha^2) \bigg\{ 4 \int_0^\infty \frac{dx}{Q^4} \frac{x^2}{1+\exp[t x - x^2 - a]} \bigg\}.
$$

Thus, if one subtracts the Coulomb potential $V_C(r)$ from $V_{\text{eff}}(r)$:

$$
V_{\text{eff}}(r) - V_C(r) = -\frac{2Ze^2}{\pi} k_F \int_0^\infty \frac{dQ}{Q} \frac{\sin(Qk_Fr)}{(Qk_Fr)} \left[ \frac{1}{1+t^2(Q, n, t)/Q^2} \right].
$$

Then, by virtue of (48), the factor in the parenthesis vanishes from large $Q$ as $\frac{1}{Q^4}$. Thus, one needs to evaluate
(49) only up to some large $Q_{\text{max}}$ (typically about 100) to obtain $V_{\text{eff}}$:

$$V_{\text{eff}}(r,n,t) \sim -\frac{Ze^2}{r} - \frac{2Ze^2}{n} k_F \int_0^{Q_{\text{max}}} dQ \frac{\sin(Q k_F r)}{(Q k_F r)} \left[ \frac{1}{1 + \frac{Z^2}{Q^2}(Q,n,t)/Q^2} - 1 \right]$$  \hspace{1cm} (50)$$

This facilitates the computation a great deal. For each set of values of density and temperature, $V_{\text{eff}}$ is computed as a function of $r$ using eq. (50) and (32) in conjunction with (30). In actual calculation, numerical fits are made to $V_{\text{eff}}(r)$ and the radial Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2mr^2} + V_{\text{eff}}(r,n,t) = E_{n\lambda} R_{n\lambda}(r)$$  \hspace{1cm} (51)$$

solved by Numerov method to obtain the energy levels. Screening lifts the $l$-degeneracy characteristic of the Coulomb potential but the $m$-degeneracy is retained as in any spherically symmetric potential. The states are labeled $(n,l)$ and the number of nodes in the radial wave function is $(n-l-1)$.

We first describe an application of the schemes to study the bound-energy levels supported by a hydrogen-like neon ion ($Z=10$) in a dense, hot plasma. Neon atoms are frequently used as probes in high temperature, dense plasmas for diagnostic purposes. Representative values of temperature and density have been chosen so as to be appropriate for laser produced plasmas.
Before discussing the spectrum, some interesting feature of $V_{\text{eff}}$ should be noted. The full momentum dependence and statistical-mechanical degeneracy effect combine to make $V_{\text{eff}}$ deeper in general than the SSCP. This is shown in Fig. 3a, b for $T$ and $n$ such that $t \geq 1$, $V_{\text{eff}}$ exhibits oscillations for $r > 5.5a_o$ while $V_\zeta$ and $V_D$ are smooth. At large $r$, $V_\zeta$ finally merges with $V_{\text{eff}}$. $V_\zeta$ generally lies lower than $V_D$. Because of oscillations, they cross $V_{\text{eff}}$ as seen from the figure 3a. For $t > 1$, $V_{\text{eff}}$ lies lower than $V_\zeta$ over the entire $r$-range (Fig. 3b).

Fig. 3c shows a plot of $V_{\text{eff}}$ as a function of $r$ for three different densities at a fixed temperature $T=100$ eV. For these densities, the parameter $t$ corresponds to 1, 1.5, and 2.74, respectively. The spatial oscillations in the potential are seen to get reduced as $t$ increases, eventually becoming a smooth potential. These oscillations are the remnants of the Friedel oscillations in the degenerate limit which arises from the sharp Fermi sphere of the electron gas at $t=0$. The blurring of the Fermi sphere at a finite temperature reduces the oscillations, eventually producing a smooth potential at high $t$. The damping of the Friedel oscillations at finite temperatures has been theoretically discussed before by Gouedard and Deutsch.

Table 4 displays the 1s, 2s, 2p energy levels along with the line shifts for three different plasma densities,
corresponding to \( t = 1, 1.5, \) and 2.74. For comparison, the corresponding results obtained using the Debye potential and \( V_\zeta(r) \) are also tabulated. This shows that the spectrum obtained with \( V_{\text{eff}} \) is substantially different from that given by the Debye theory. As anticipated, the higher levels are much more affected than the 1s-level. For \( n = 4.54 \times 10^{24} \text{ cm} \ (t=1) \), the 2s-level is deeper by 39\% and 2p-level by as much as 62\% compared to the Debye values. While the statistical mechanical degeneracy effect accounts for more than 50\% of this difference the full momentum dependence is also seem to make a very significant contribution. The difference with the Debye spectrum gradually decreases as \( t \) gets larger. At \( t = 2.74 \), the major difference is due to Q-dependence of \( V_{\text{eff}} \).

More importantly, the line shifts (measured relative to the unscreened Coulomb value of 75 Ryd.) are found to be substantially smaller than those obtained from the Debye theory. The Lyman \( \alpha \)-line shifts (2p\( \rightarrow \)1s transition) is reduced by about 50\% and is quite sensitive to plasma density. Since the total transition probability in the electric dipole approximation is given by

\[
A_{n\ell, n'\ell'} = \frac{4e^2}{3\hbar c^3} |\langle n\ell | \hat{r} | n'\ell' \rangle|^2 \left| \frac{E_{n\ell} - E_{n'\ell'}}{\hbar} \right|^3.
\]

The intensity of the radiation emitted is affected substantially. It is for this reason, this shift is important for plasma diagnostics.
To study the temperature dependence of the energy eigenvalues, another set of calculations at $T = 750$ eV is presented in Table 5. Here, because of large $t$-values, $V_\zeta(r)$ merges with $V_D(r)$ and the difference in energy levels is entirely due to $Q$-dependence of $V_{\text{eff}}$. Note that although differences in energy levels are small, the line shifts are still about 20-30% smaller than the Debye values.

Fig. 4 shows the spectra at the two temperatures considered as a function of density. For each temperature, as the density increases, the spectrum shifts upward. Since the screening effect increases, the higher levels move up faster than the ground state. For the same density, the energy levels are deeper at higher temperatures, because temperature weakens screening and thus the associated shifts are reduced. Comparison of Tables 4 and 5 shows that $2p - 1s$ separation for a given density increases as the temperature increases, since a reduction in screening makes the spectrum more like that of unscreened coulomb potential.

For the same density range and at $T = 750$ eV, Skupsky has recently presented a calculation of the spectrum for neon. In his scheme, he solves the Poisson eq. self-consistently to obtain an effective potential which includes the contribution of both bound and free electrons. Although there are several approximations in his scheme, it clearly goes beyond the linear screening theory. Interest-
ingly, however, the line shifts (Fig. 5) and the breaking of the coulomb degeneracy (Table 5(b)) (needed for line profile calculations) we obtain are in reasonable agreement with his results. At the highest density we have considered \((n = 4.56 \times 10^{24} \text{ cm}^{-3})\), our result is very close to his; in fact, our scheme gives better results than the other models he used for comparison, as shown in Tables 5a and 5b.

Another model potential that is frequently used in estimating plasma screening effect is the Ion-sphere model (Stewart and Pyatt)\(^{16}\):

\[
V_{\text{IS}}^{\text{SP}} = -\frac{Ze^2}{r} + \frac{(Z-1)e^2}{2R_o} \left[3 - \left(\frac{r}{R_o}\right)^2\right], \quad r \leq R_o
\]

\[
= 0, \quad \text{otherwise}
\]

Here \(R_o = \left(\frac{3}{4\pi}\right)^{1/3} \left(\frac{Z-1}{n}\right)^{1/3}\) is the ion-sphere radius. We observe that \(V_{\text{IS}}\) could be obtained very simply from the sum of Coulomb and Hartree potentials:

\[
V_{\text{IS}}(r,n) = -\frac{Ze^2}{r} + e^2 \int \frac{\rho(r')}{|\mathbf{r} - \mathbf{r}'|} dr'.
\]

with

\[
\rho(r') = n \quad \text{for} \quad r' \leq R_o
\]

\[
= 0 \quad \text{outside}
\]

and \(R_o\) is chosen such that \(4\pi \int_0^{R_o} r'^2 \rho(r') = (Z-1)\).
Then, by performing the indicated integration in eq. (53), we get eq. (52) for \( r \leq R_0 \). But for \( r \geq R_0 \), we obtain

\[
V_{IS} = -\frac{e^2}{r}, \quad r \geq R_0.
\]  

(54)

Physically, this model assumes a smeared out uniform electron density distribution \( n \) within a sphere and zero density outside the sphere. The radius of the sphere is adjusted so that the total amount of charge inside the sphere, by construction, is that of a singly ionized ion. The electrostatic potential outside this uniformly charged sphere is thus naturally \(-\frac{e^2}{r}\), as given by eq. (54). On the other hand, in the ion-sphere model (Stewart and Pyatt), the potential outside the sphere is set equal to zero at \( r = R_0 \). (Let us note, in passing, for a multiply-ionized atom, one simply has to set \( \int \rho(\mathbf{r}') \, d^3\mathbf{r}' = (Z-m) \) with \( m = 2 \) for doubly-ionized etc. In such cases, \( V_{IS} = -\frac{me^2}{r} \)

for \( r \geq R_0 \).

When (52) and (53) are used to compute the neon spectrum (Table 6) by numerical solution of the Schrödinger equation, the results are significantly different from the lowest order perturbation calculation given by Skupsky\textsuperscript{11} using the Stewart-Pyatt potential \( V_{IS}^{SP} \). Again, the line shift and the breaking of the coulomb degeneracy (Table 5a, 5b obtained from our \( V_{eff} \) are closer to Skupsky's self-consistent results than those obtained using the Ion-
sphere model presented above (Table 6). The 2p-ionization potential using $V_{\text{eff}}$ (Table 5) are also much closer to the self-consistent values (Fig. 1 of Skupsky) than the corresponding results from eqs. (52) and (53).

IV. Screening of impurity states in a semiconductor

There has been a good deal of interest, both theoretical and experimental, in the properties of shallow impurity states (acceptors and donors) in semiconductors in recent years. In contrast to high density laser-produced plasmas, the doped semiconductors represent low density systems: Highly doped semiconductors at room temperatures; however, correspond to the "intermediate degeneracy situation". As an example of free-carrier concentration $n_e = 6.7 \times 10^{18}$ cm$^{-3}$, the room temperature $T = 300^\circ$ K corresponds to $t \sim 2$ (assuming effective mass $m^* = m_e$). The screening model we developed earlier in this chapter could therefore be fruitfully employed to study the screening of impurity states in semiconductors in such conditions.

For the case of very low impurity concentration, each impurity site can be treated as an isolated center. Then, within the effective-mass approximation, the effective interaction between the conduction electron and the central ion of the impurity atom is taken to be Coulombic in nature. Kohn and Luttinger$^{17}$ and some other workers$^{18}$ have solved the impurity Hamiltonian in this approximation using hydrogenic trial wave function in a varia-
tional calculation. However, for high impurity concentration, one finds significant overlap between the electronic wave functions of neighboring impurity atoms. This overlap allows an appreciable fraction of these electrons to become relatively mobile. The presence of these free carriers modifies the simple Coulombic electron-ion interaction—giving rise to the screening effect.

Traditionally, such screening effects for impurity states in a semiconductor has been investigated by Thomas-Fermi potential\textsuperscript{19,20}. The Lindhard\textsuperscript{20,21} and the Hubbard-Sham\textsuperscript{20,22} screened potentials have also been used to study the binding energy of an electron bound to a donor impurity. Only the ground state has been studied by means of a variational calculation. In the present work, we investigate the ground-state as well as the higher lying states by direct numerical integration of the relevant Schrödinger equation. The effect of temperature is explicitly included via the finite temperature RPA-screened potential. As we shall see below, the spectrum of impurity states at room temperature could be significantly different from what is obtained by using zero temperature screening.

Debye screening has been used by Rogers, et al.\textsuperscript{24} and others\textsuperscript{23} to investigate screening effects of impurity charges in an electron gas at finite temperatures. Depending on the electron density, however, 'intermediate degeneracy' situation can occur and appropriate degeneracy
effect should be considered via the $V_\zeta$-potential. These effects are important, particularly for higher impurity states. This is illustrated by the results of the calculation presented in Table 7. Here we study the spectrum of bound states due to a singly charged impurity ($Z = 1$) embedded in an electron gas at $T = 300^\circ K$, as a function of electron density. The three different densities chosen are typical of a highly doped semiconductor and the corresponding $t$-values fall within the 'intermediate degeneracy' region. As seen from Table 7, the energy level spectrum supported by $V_\zeta$-potential is significantly different from the corresponding Debye potential. The effects are more substantial, for higher lying states. For $n = 10.28 \times 10^{18}$ electrons/cm$^3$ ($t = 1.5$), the 2p-state in the $V_\zeta$-potential is deeper by about 20%. As the density increases, the higher lying states are pushed out to the continuum due to increased screening effects. Note that the number of bound states are different in the two potentials. A shallow 3d-state still exists for the $V_\zeta$-potential for $n = 6.67 \times 10^{18}$ cm$^{-3}$ but not in the Debye potential since $V_D(r)$ overestimates the screening effects.

Next, we consider an application of the above scheme to screened donor impurity states in Silicon, at room temperature, within the isotropic effective mass approximation. Only singly charged donor impurities are consi-
dered: for example, Phosphorous in Silicon. The dielectric constant of the material \( K = 11.8 \) must be considered, so that the effective impurity potential \( V_{\text{eff}}(r,n,t) \) is given by

\[
V_{\text{eff}}(r,n,t) = -\frac{e^2}{K r} - \frac{2e^2}{\pi K} k_F \int_0^\infty dQ \frac{\sin(Q k_F r)}{(Q k_F r)} \left[ \frac{1}{1 + \xi^2(Q,n,t)/Q^2} - 1 \right]
\]

(55)

It is convenient to measure lengths in units of 'effective' Bohr radius \( a = K a_0 \) and energies in 'effective' rydberg \( = e^2/(2aK) \). For different densities \( T = 300^\circ \text{K} \), \( V_{\text{eff}}(r,n,t) \) is directly computed in \( r \)-space (eq. (55)). The discrete values of \( V_{\text{eff}}(r) \) are fitted by using cubic splines, and used in the radial Schrödinger equation to solve for the bound-state energy levels by numerical integration (Numerov method). The carrier concentrations chosen are typical of highly doped semiconductors. Results of these calculations are given in Table 8. For comparison, the corresponding bound-state spectrum obtained using the Thomas-Fermi, Debye and \( V_\zeta \)-potentials are also tabulated. Since optical properties of semiconductors are of interest 1s \( \rightarrow \) 2p level spacings are also listed.

For each of the three different densities we have chosen, the effect of full momentum dependence and appropriate degeneracy effect combines to make \( V_{\text{eff}} \) the deepest
of all the four potentials. The corresponding bound-state spectrum due to \( V_{\text{eff}} \) is thus significantly deeper than that due to the other potentials. The zero temperature approximation, \( V_{TF} \), of course, severely overestimates the screening effect and does not support 2s or 2p- states in this density range.

The impurity level spectrum, particularly the higher state, is seen to be very sensitive to carrier concentration. The 2p level in \( V_{\text{eff}} \) changes from -0.014 effective Ryd. to -0.006 effective Ryd., as the carrier density increases from \( 1.69 \times 10^{18} \ \text{cm}^{-3} \) to \( 1.98 \times 10^{18} \ \text{cm}^{-3} \). This is due to the fact that these impurity states are very shallow (or weakly bound) and therefore very sensitive to screening effects.

As the carrier density increases, the spectrum of states move upwards due to increased screening effects. However, the rate at which the energy levels move up is much faster when Thomas-Fermi potential is used instead of the appropriate \( V_{\text{eff}} \). If the carrier density exceeds a critical value, \( n_c \), even the lowest 1s bound state is pushed out to the continuum. Thus the activation energy vanishes beyond this critical density \( n_c \). This, of course, is the familiar Mott transition. Mott\(^{19}\) was the first to point out that this vanishing of the activation energy would result in an abrupt insulator to metal transition. However, he assumed TF-screening to estimate \( n_c \) and obtained
Variational calculation with hydrogenic trial function using Lindhard dielectric screening at zero temperature and assuming isotropic mass approximation was done by Greene\textsuperscript{20} et al. His result is

\[ a_{c}^{1/3} \approx 0.29 \]  

(57)

This is expected since the Lindhard-screened potential is substantially deeper than the TF-potential for the same density and therefore predicts higher density for the removal of the last bound state. (Let us note here that Krieger and Nightingale\textsuperscript{21} who first estimated the Mott criterion by the above method obtained \( a_{c}^{1/3} \approx 0.23 \). However, the calculation of Ref. 20 is consistent with eq. (56) and also with the result obtained by Rogers\textsuperscript{24} et al. by numerical integration of Schrödinger equation using SSCP.)

A parallel variational calculation by us using the temperature dependent Lindhard dielectric function with hydrogenic trial function gives

\[ a_{c}^{1/3} \approx 0.31 \]  

(58)

which is slightly higher than the zero temperature result, eq. (57). This, of course, is expected and could be understood as follows: eq. (57) predicts a critical density \( n_{c} \approx 10^{20} \) electron/cm\(^3\), so that room temperature \( T = 300^\circ K \)
corresponds to $t$ of about 0.3. Thus, the temperature effect reduces the screening effect slightly, producing a deeper potential. However, the difference is quite small.

Thus, the critical density moves to a slightly higher value so that the screening is just sufficient to remove the last bound state.

The experimental result of Alexander and Holocomb\cite{Alexander} seems to predict a substantially lower critical density $n_c^{1/3} \approx 0.22$. As pointed out by Greene\cite{Greene}\ et al., the hydrogenic trial function is not very adequate in this case. Their calculation using Hülthen trial function with appropriate valley degeneracy (4 for Silicon) improved the Mott criterion substantially: $n_c^{1/3} \approx 0.27$. Further calculation by Aldrich which includes the Silicon mass anisotropy gives $n_c^{1/3} \approx 0.25$. Let us note here that a self-consistent LDA-calculation has also been performed by Rose, Shore and Sander\cite{Rose} which predicts a metal-insulator transition at a much higher density ($n_c \approx 10^{22}$ cm$^{-3}$).

From the results presented so far, we see that useful estimates of the energy levels, line shifts etc., could be obtained using the temperature dependent Lindhard screened potential as a model impurity potential in dense, hot plasmas as well as semiconductor
materials. The density and temperature dependence are included in this scheme in a natural way, in contrast to the Ion-sphere model. In the intermediate degeneracy region, the screening effect is grossly over-estimated by the Debye theory. It is in this region that our scheme is most useful.

As pointed out before, no exchange-correlation effects have been considered in this scheme. These effects will be investigated in detail in the following chapters.
CHAPTER III

EXCHANGE EFFECTS FOR ELECTRON SYSTEMS AT FINITE TEMPERATURES

In the previous chapter, an approximate form of Kohn-Sham effective potential was used to describe the screening effects at finite temperatures. All exchange-correlation effects were neglected, as a first approximation, to obtain this screened potential. In this and the following chapter, we investigate these many-body effects in detail. This is needed, as emphasized earlier, for a systematic generalization of the local density functional theory to finite temperatures.

In the 'local' approximation to density functional theory (L.D.A.), the density profile corresponding to the inhomogeneous system is considered to be 'piecewise' or 'locally' uniform. The properties of the homogeneous interacting electron gas could then be used as input data to study the inhomogeneous system. At zero temperature, a calculation of the exchange-correlation energy $E_{xc}[n]$ for various densities is used to set up the exchange-correlation potential $V_{xc}[n]$ by taking the functional derivative: $V_{xc} = \delta E_{xc}/\delta n$. At finite temperatures, $\Omega_{xc}[n,T]$ plays the same role as $E_{xc}$ at $T = 0$, and the corresponding exchange-correlation potential depends both on density and temperature, given by $V_{xc}[n,T] = \delta \Omega_{xc}[n,T]/\delta n$. 

45
Let us note here that in several previous works, a zero temperature $V_{xc}[n]$ has been employed in solving finite temperature Kohn-Sham equations. In such schemes, the temperature dependence is brought in only through the expression for local density, equation (18c). However, the explicit additional temperature dependence of $V_{xc}[n,T]$ itself is very important, as we shall see later on.

In this chapter, we will discuss the exchange effects only. A detailed investigation of correlation effects will be taken up in the next chapter.

An exact treatment of exchange effects requires the solution of the full Hartree-Fock integro-differential equation. The task is enormously simplified by the 'local density' approximation to the non-local Hartree-Fock exchange operator. Within this approximation, the local exchange potentials $V_x^S = -\frac{3}{2} \frac{e^2}{\pi} [3n^2 n(r)]^{1/3}$ of Slater \cite{28} and $V_x^{KS} = \frac{2}{3} V_x^S$ of Gaspar-Kohn-Sham \cite{1} have been extensively used for a variety of atomic and solid state calculations. The difference in the prefactor is due to the fact that only the states at the top of the Fermi level are considered to obtain the Gaspar-Kohn-Sham potential whereas averaging over all the occupied states leads to the Slater potential. As argued by Kohn and Sham, $V_x^{KS}$ is physically more appealing, since the density adjustments come about by redistribution of electrons near the Fermi
level. Moreover, $V^{KS}_x$ is a consequence of a variational principle whereas $V^S_x$ is not, as was shown by K-S.

The Kohn-Sham exchange potential (as also $V^S_x$) is really valid only at $T = 0^\circ K$. A finite temperature generalization of $V^{KS}_x$ is needed for application to a variety of plasma conditions, particularly for intermediate degeneracy situation.

Consider an interacting homogeneous electron gas of density $n$ in thermal equilibrium at a temperature $T$. Let $\Omega_o[n,T]$ be the grand potential for a non-interacting system of electrons at the same density and temperature. Then, for the interacting electron gas, by using finite temperature field theoretic formalism, one can show that the grand potential $\Omega[n,T]$ is given by

$$\Omega = \Omega_o + V^S_x \int_0^1 \frac{d\lambda}{\lambda} \int \frac{d^3k}{(2\pi)^3} \frac{1}{\beta \hbar n} \sum e^{i\omega_n\delta} \frac{H}{Z} \frac{e^{*\lambda}(k,\omega_n)G^\lambda(k,\omega_n)}{\sum_{\lambda}} + \Omega_{xc},$$

where $\beta = (k_B T)^{-1}$, $V_o$ is the volume of the system and $e^{i\omega_n\delta}$ is a convergence factor with $\lim \delta \to 0^+$ implied. $\Sigma^*(k,\omega_n)$ is the 'proper' self-energy defined via the Dyson equation for Green's function for the interacting electron system:

$$G(k,\omega_n) = G_o(k,\omega_n) + G_o(k,\omega_n)\Sigma^*(k,\omega_n) G(k,\omega_n),$$

where $G_o(k,\omega_n)$ is the temperature Green's function for non-
interacting electrons:

\[ G_0(k, \omega_n) = \frac{1}{i\omega_n - \mu^{-1}(\epsilon_k - \mu)}; \quad \epsilon_k = \frac{\hbar^2 k^2}{2m}, \quad (61) \]

and \( \mu \) is the chemical potential. Apart from the usual momentum \((k)\) dependence, the temperature Green's function for fermions depends also on the discrete 'frequencies'

\[ \omega_n = (2n+1)\pi/\beta \hbar \quad (n = +\text{ve or } -\text{ve integers}), \]

because of the antiperiodicity of \( G \) in the time variable in the range \((0, \beta \hbar)\).

Equation (59) above is an exact expression and defines the exchange-correlation contribution to the grand potential, \( \Omega_{xc} \). An integration over the variable coupling parameter \( \lambda \) is needed; \( \lambda = 0 \) corresponds to the non-interacting system whereas \( \lambda = 1 \) represents the actual physical system. In practice, it is necessary to make suitable approximations to the \( G^\lambda \) and \( \Sigma^\lambda \) in order to evaluate \( \Omega_{xc} \). The scheme we employ here is to include the first-order exchange and the sum of 'ring'-diagram contributions to take into account some of the correlation effects, i.e.,

\[ \Sigma^*(k, \omega_n) \approx \Sigma^*(1) (k, \omega_n) + \Sigma^x (k, \omega_n) \quad (62) \]

so that

\[ \Omega_{xc} \approx \Omega_x + \Omega_c^{(r)} \quad (63) \]

The rest of the discussion in this chapter is on exchange effects only. The ring-diagram contribution will be investigated in the following chapter. An estimate of the
Second order exchange contribution is given in Appendix B.

The first-order exchange contribution to proper self-energy, $\Sigma_x^*(1)$, can be evaluated with the Feynman rules to give

$$\Sigma_x^*(1)(k) = -\int \frac{d^3k'}{(2\pi)^3} \frac{1}{\beta\xi} \sum_{\eta} e^{i\omega_{n',\eta}} V(k-k') G^0(k',\omega_{n'})$$

(64)

where $V$ is the Fourier transform of the bare Coulomb interaction and $G^0$ is given by eq. (61). The frequency sum is of the form $\sum_{\eta=0}^{1} \frac{i\omega_{n',\eta}}{\eta}$ and can be evaluated by usual contour integration to obtain the fermi function

$$f(k) = \frac{1}{[e^{\beta(\epsilon_k-\mu)} + 1]}$$

$$\lim_{n \to 0^+} \sum_{n \text{ odd}} \frac{i\omega_{n',\eta}}{\eta} = \frac{\beta\xi}{\epsilon_{k'} - \mu} + 1$$

(65)

Therefore

$$\Sigma_x^*(1)(k) = -\int \frac{d^3k'}{(2\pi)^3} V(k-k') f(k')$$

(66)

The corresponding contribution to Grand potential is

$$\Omega_{x} = -\int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} V(k-k') f(k) f(k')$$

(67)

The purposes of analysis and computation, it is convenient to scale all momenta by the Fermi momentum

$$k_F = (3\pi^2n)^{1/3}: k = xk_F, k' = yk_F.$$
carrying out the angular integration, is
\[ \Omega_x[n,T] = \Omega_x[n,0] \cdot I(t) \] (68)
where
\[ \Omega_x[n,0] = \frac{e^{2k_F^2}}{4\pi^3}, \] (69)
which is the usual zero temperature Hartree-Fock exchange energy for an electron gas of density \( n \) and
\[ I(t) = 2 \int_0^\infty \int_0^\infty dx \, dy \, x f(x) y f(y) \ln \left| \frac{x+y}{x-y} \right|, \] (70)
with
\[ f(x) = \frac{1}{1 + \exp[t^{-1} x^{2-\alpha}]} \] (71)
The degeneracy parameter \( \alpha = \beta \mu \) is determined from the condition that the total number density is fixed,
\[ n = 2 \int \frac{d^3k}{(2\pi)^3} f(k) \]
or
\[ \frac{2}{3} t^{-3/2} = \int_0^\infty dx \, x^{1/2} \frac{x}{\exp(x-\alpha) + 1} \] (72)
At any given density \( n \) and temperature \( T \), the ratio \( t = T/T_F \) fixes the degeneracy parameter \( \alpha \) by eq. (72) and thus also \( f(x) \) and \( f(y) \). The two-dimensional integral \( I(t) \) in eq. (70) thus depends only on \( t \), and not separately on \( n \) and \( T \).

For the exchange-potential \( V_x = \frac{\delta \Omega_x}{\delta n} \), we obtain
\[ V_x[n,T] = V_x[n,0] \cdot F(t) \] (73)
where \( V_x[n,0] = -\frac{e^2}{\pi} (3\pi^2 n)^{1/3} \) is the usual Kohn-Sham exchange potential and

\[
P(t) = \int_0^\infty \int_0^\infty dx \, dy \, x \, f(x) \, y \, f(y) \, (1-f(y)) \ln \frac{|x+y|}{|x-y|} \quad . \tag{74}
\]

In obtaining (74), we note that

\[
\frac{d}{da} f(x) = f(x) (1-f(x)) ,
\]

and \( \frac{da}{dn} \) is obtained from (72) as

\[
\frac{da}{dn} = \frac{1}{\frac{\kappa_F^3}{3\pi^2} \left[ 1 - 3 \int_0^\infty dx \, x^2 \, f^2(x) \right]} .
\]

It is clear from above that the scaled quantities

\[
\frac{\Omega_x[n,T]}{\Omega_x[n,0]} \quad \text{and} \quad \frac{V_x[n,T]}{V_x[n,0]}
\]

are functions of \( t \) only. This is a special feature of this approximation. This facilitates the computation a great deal, since these scaled quantities could be directly computed as a function of \( t \), in conjunction with equations (71) and (72). The result of these calculations are given in Table 9.

The variations of these scaled quantities are represented in a very useful way via the "universal" curves: Fig. 6(a) and 6(b). These plots allow us to obtain an estimate

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
of these quantities at all relevant densities and temperatures. Only the exchange energy \( \Omega_x \) had been calculated by Cowan and Ashkin\(^ {30} \) at different densities for a few fixed temperatures.

In the limit of \( t \to 0 \), it can be shown\(^ {31} \) that

\[
I(t) \approx 1 + \frac{\pi^2}{6} t^2 \ln t + At^2 + O(t^4 \ln t, t^4), \tag{75}
\]

exhibiting a decrease initially for infinitesimal \( t \). \( A \) is a known\(^ {31} \) constant. From this, we obtain

\[
\frac{V_x[n,T]}{V_x[n,0]} \approx 1 - \frac{\pi^2}{12} t^2; \quad (t \to 0)
\tag{76}
\]

In the other limit of \( t \to \infty \), as shown by Cowan and Ashkin\(^ {30} \), (an alternative simpler way of calculating the two dimensional integral, due to Rajagopal, is given in Appendix A).

\[
I(t) \xrightarrow{t \to \infty} 2e^{2\alpha} \int_0^\infty \int_0^\infty e^{-t} (x^2 + y^2) \ln \left| \frac{x + y}{x - y} \right| dx \, dy
\]

\[
= 2e^{2\alpha} t^2 \cdot \frac{\pi}{8},
\]

with

\[
\alpha \xrightarrow{t \to \infty} \ln \left[ \frac{4}{3\pi} t^{-3/2} \right],
\]

and hence

\[
I(t) \xrightarrow{t \to \infty} \frac{4}{9t} \tag{77}
\]

Using (77), we obtain

\[
\frac{V_x[n,T]}{V_x[n,0]} \xrightarrow{t \to \infty} \frac{2}{3t}. \tag{78}
\]

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
These relations are useful in checking numerical calculations of the relevant quantities for small and large $t$ values. As seen from Table 9 and Fig. 6, the exchange potential $V_x$ weakens with increasing temperature as expected but not as rapidly as the exchange free energy, $\Omega_x$. In fact, $V_x [n,T]$ decreases quite slowly in the range $0 < t < 0.3$ and again in the high temperature region $t > 2.5$, a trend shared by $\Omega_x [n,T]$ as well. The vanishing of exchange effects at high temperatures is expected since it arises from Pauli exclusion principle.

As emphasized in the previous chapters, the domain $0.3 < t < 3.0$--the "intermediate degeneracy region"--is particularly important since neither quantum (Thomas-Fermi-type) nor classical (Debye-type) theories is applicable here. Both $V_x [n,T]$ and $\Omega_x [n,T]$ are sensitive functions of $t$ in this region as seen from their rapid variation: $V_x [n,T]$ increases from $0.25 V_x [n,0]$ at $t = 2.5$ to $0.85 V_x [n,0]$ at $t = 0.5$.

Table 10 (a)-(d) lists the values of $\Omega_x [n,T]$ per particle and $V_x [n,T]$ for several densities in the range $t = 0.1$ to 10. The densities are chosen so as to be appropriate for dense laser produced plasmas and highly doped semiconductors. Note that this range of $t$ covers the most interesting temperature region. For a low density plasma with $n = 10^{18}$ cm$^{-3}$, $T_F = 42.3$ K; a temperature of $T = 1 \text{ eV} \sim 10^4$ K is extremely high, so that exchange

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
effects practically disappear. However, for a superdense laser imploded plasma of \( n = 10^{26} \text{ cm}^{-3} \), \( T_p = 9 \times 10^6 \text{ K} \); the same temperature of \( T = 1 \text{ eV} \) is practically zero temperature for such a plasma and exchange effects are very important. The relevance of this range of \( t \) for different densities will be seen more clearly in connection with correlation effects in the next chapter.

The rapid increase of both \( \Omega_x \) and \( V_x \) with density should be noted from the tables 10 (a)-(d) indicating the importance of exchange effects at high densities. For example, \( V_x \) increases from -0.056 Ryd. for \( n = 10^{22} \text{ cm}^{-3} \), \( t = 2.5 \) to as much as -0.262 Ryd for \( n = 10^{24} \text{ cm}^{-3} \) for the same \( t \). Note that in maintaining \( t = 2.5 \), the temperature has to be correspondingly changed as we go from one density to the other. However, this importance would be grossly overestimated if the temperature effects were not properly included (as in the zero temperature, \( \rho^{1/3} \)-theory).

The \( V_x[n,T] \) presented here represented the generalization of the traditional \( \rho^{1/3} \)-theory for all temperatures. A detailed investigation of correlation effects will be taken up in the following chapter in order to obtain the full exchange-correlation potential, \( V_{xc}[n,T] \).
CHAPTER IV

ELECTRON CORRELATIONS AT FINITE TEMPERATURES

In this chapter, we investigate the electron correlation effects at finite temperatures due to the 'ring' diagram contributions. For applicability to plasmas in a wide variety of conditions, one has to consider broadly the following regions: (1) low temperature, low density; (2) low temperature, high density; (3) high temperature, low density; and (4) high temperature, high density. A fully satisfactory treatment of correlation effects valid for all the different regions is a formidable task. However, we give below the reasons why the 'ring' diagram contributions could be expected to be an adequate scheme for all but the first one of the regions mentioned above.

Firstly, in region (2), some exact results are known. This is the 'weak coupling' domain—the average potential energy per electron is a weak perturbation on the average kinetic energy. Thus, a diagrammatic perturbation theory could be applied to calculate the correlation energy. At zero temperature, Gell-Mann and Brueckner showed that the sum of 'ring' diagrams, being the most divergent set of diagrams, gives the asymptotically exact result in the high density limit.

At zero temperature, for low or intermediate densities, the 'weak coupling' scheme does not hold. At very low den-
sities, potential energy dominates over kinetic energy. This 'strong coupling' situation results in localizing the electrons to form a Wigner lattice. An approach very different from that of the 'ring'-diagrams was used by Wigner\textsuperscript{33} to estimate the correlation energy of a low density electron gas at T=0.

For intermediate densities at zero temperature, the kinetic energy and the potential energy play roughly comparable roles in determining the electron behavior. Interpolation formulas, by Wigner\textsuperscript{33}, Nozi\'ers and Pines\textsuperscript{34}, etc., have been used to obtain the correlation energy in this situation. Although there is no obvious reason to expect the 'ring'-approximation to work well in this domain, Pines and Nozi\'ers\textsuperscript{34} showed that the contribution to correlation energy from small momentum transfers are still accurately obtained from the ring-diagrams. Also, at very low densities, Iwata\textsuperscript{35} showed that the same set of 'ring' diagrams reproduces the first two terms of Nozi\'ers and Pines result, obtained by a very different approach, namely the extended Bohm-Pines Hamiltonian. These facts encourage us to use ring-diagrams in the intermediate densities as well. In fact, the most commonly used expressions for $E_{xc}$ and $V_{xc}$ at T=0 is that due to von Barth and Hedin\textsuperscript{36} which is based on the numerical evaluation of the sum of 'ring'-diagram contributions in the metallic density range.
For low densities and high temperature, the 'weak coupling' scheme becomes applicable again. The reason is that the average kinetic energy increases with temperature whereas the potential energy decreases. In region (4), a perturbation approach is again valid.

It was Montroll and Ward who obtained the free energy of the electron gas at $T \neq 0$ in terms of a diagrammatic perturbation series. In region (3), exact results are known in fact, DeWitt showed that for low densities in the $T \to \infty$ limit, the classical Debye-Hückel result for the correlation contribution to free energy is obtained from the 'ring' diagram sum. Kraft et al. have also used the 'ring' diagram to evaluate the correlation energy for densities and temperatures appropriate for gaseous and solid state plasmas.

As mentioned before, the infinite series of terms in the 'ring' sum consists of the most divergent diagrams in each order of the perturbation series. The source of the divergence is the occurrence of the same momentum transfer on each interaction line and the associated coulomb interaction. The effective two-body interaction in the 'ring' approximation is given by

$$V_r(q, \nu_n) = \frac{V(q)}{1 - V(q) \chi(q, \nu_n)}$$

($V(q) = 4\pi e^2/q^2$)
where $\chi(q,\nu_n)$ is the 'proper' polarization and is given by

$$\chi(q,\nu_n) = \frac{2}{\beta \hbar^2} \sum_{\omega_1} \int \frac{d^3p}{(2\pi)^3} \frac{1}{\beta \hbar} \omega_1 \left[ \frac{1}{i\omega_1 - \hbar(\epsilon_p - \nu)} \right] \left[ \frac{1}{i\omega_1 + i\nu - \hbar(\epsilon_{p+q} - \nu)} \right] G^0(p,\omega_1) G^0(p+q,\omega_1+\nu_n)$$

$$= \frac{2}{\beta \hbar^2} \sum_{\omega_1} \frac{d^3p}{(2\pi)^3} \frac{1}{\beta \hbar} \omega_1 \left[ \frac{1}{i\omega_1 - \hbar(\epsilon_p - \nu)} \right] \left[ \frac{1}{i\omega_1 + i\nu - \hbar(\epsilon_{p+q} - \nu)} \right] G^0(p,\omega_1) G^0(p+q,\omega_1+\nu_n)$$

$$(\epsilon_p = \hbar^2 p^2 / 2m)$$

The frequency sum is done by the usual contour-integral method to yield

$$\chi(q,\nu_n) = -2 \int \frac{d^3p}{(2\pi)^3} \frac{f(p+q) - f(p)}{i\hbar \nu_n - (\epsilon_{p+q} - \epsilon_p)}$$

(80)

with $\nu_n = \frac{2n\pi}{\beta \hbar}$, $(n = + \text{ve integers})$.

We note from (79) that the effective interaction is no longer the bare coulomb interaction but is screened by the factor $[1-V(q) \chi(q,\nu_n)]^{-1}$ which represents the effect of the polarization of the surrounding medium—that is, each electron is surrounded by its polarization cloud. The analytic continuation of $\chi(q,\nu_n)$ is the polarization or response function $\chi(q,\nu)$. The static $(\nu=0)$ part of this
function was used in Chapter II to describe screening effects.

To obtain the correlation contribution to the thermodynamic potential, one needs to evaluate the 'ring' contribution to the proper self-energy,

\[
\Sigma^*_\lambda (k, \omega_n) = -\frac{1}{\beta} \int \frac{d^3q}{(2\pi)^3} \frac{1}{\beta\hbar} \sum_{\nu_n} [V(q, \nu_n) - V(q)] G^0(k - q, \omega_n - \nu_n)
\]

\[
= \frac{1}{\beta\hbar^2} \int \frac{d^3q}{(2\pi)^3} \sum_{\nu_n} \frac{[V(q)^2 \chi(q, \nu_n)]}{1 - V(q) \chi(q, \nu_n)} G^0(k - q, \omega_n - \nu_n)
\]

(81)

Note that the part associated with the bare coulomb potential \(V(q)\) in the first expression above corresponds to the exchange contribution and thus has to be subtracted off.

The 'ring' contribution to the grand potential is

\[
\Omega_c^{(e)} = \frac{V_0}{\beta} \int \frac{d\lambda}{0} \int \frac{d^3x}{(2\pi)^3} \sum_{\nu_n} \frac{\ln \chi(q, \nu_n)}{\omega_n} \Sigma^*_\lambda (k, \omega_n) G^0(k, \omega_n)
\]

\[
= \frac{V_0}{2\beta} \sum_{\nu_n} \int \frac{d^3q}{(2\pi)^3} \int \frac{d\lambda}{0} \frac{[\lambda V(q) \chi(q, \nu_n)]^2}{1 - \lambda V(q) \chi(q, \nu_n)}
\]

\[
= \frac{V_0}{2\beta} \int \frac{d^3q}{(2\pi)^3} \sum_{\nu_n} \ln \left[1 - V(q) \chi(q, \nu_n)\right] + V(q) \chi(q, \nu_n)
\]

(82)

where \(V_0\) is the volume of the system.

From (82), we obtain the corresponding correlation potential.
\[ v_c(n, T) = -\frac{e^2}{\pi} (3\pi^2 n)^{1/3} \frac{1}{\beta} \int_{-\infty}^{\infty} \frac{d\omega}{\omega} \left[ \frac{V(Q) \chi(Q, \nu_k)}{1 - V(Q) \chi(Q, \nu_k)} \right] \frac{d\chi(Q, \nu_k)}{dn} \]

where

\[ V(Q) \chi(Q, \nu_k) = -\frac{2}{(\pi a_0 k_F)} \int_0^\infty dx x f(x) \ln \left( \frac{4\xi^2 \pi^2 x^2 + (Q^2 + 2QX)^2}{4\xi^2 \pi^2 x^2 + (Q^2 - 2QX)^2} \right) \]

and \( d\chi(Q, \nu_k)/dn \)

\[ = \frac{3\pi^2}{k_F^3} \frac{1}{[1 - 3 \int_0^\infty dx x^2 f^2(x)]} \left( \chi(Q, \nu_k) + \frac{mk_F}{2\pi^2 \hbar^2} \int_0^\infty dx x f^2(x) \ln \left( \frac{4\xi^2 \pi^2 x^2 + (Q^2 + 2QX)^2}{4\xi^2 \pi^2 x^2 + (Q^2 - 2QX)^2} \right) \right) \]

In (84), all momenta have been scaled by \( k_F \); and \( t = T/T_F \) as before.

Let us remark at this point that the discrete frequency sum could be converted into an integral form to give

\[ \frac{\Omega_C}{V_O} = \frac{mk_F}{(2\pi)^3} \int_0^{2\pi} \frac{d^3Q}{(2\pi)^3} \int_0^{2\pi} \frac{d\omega}{(2\pi)} \coth \frac{\delta \hbar \omega}{2} \left\{ \tan^{-1} \left( \frac{V(Q) \Im \chi(Q, \omega)}{1 - V(Q) \Re \chi(Q, \omega)} \right) - V(Q) \Im \chi(Q, \omega) \right\} \]
with

\[ \text{Re} \chi(Q, \omega) = \frac{m}{2\pi^2 \hbar k_F Q} \int_0^\infty dk k f(k) \]

\[
\left\{ \begin{array}{l}
\frac{\omega + \hbar k_F Q^2}{2m} - \frac{\hbar k_Q k_F}{m} \\
\frac{\omega + \hbar k_F Q^2}{2m} + \frac{\hbar k_Q k_F}{m} \\
\frac{\omega - \hbar k_F Q^2}{2m} - \frac{\hbar k_Q k_F}{m} \\
\frac{\omega - \hbar k_F Q^2}{2m} + \frac{\hbar k_Q k_F}{m}
\end{array} \right. 
\]

(86)

and \( \text{Im} \chi(Q, \omega) = \frac{m^2}{(2\pi)^4 \hbar^4 k_F Q} \)

\[
\left\{ \begin{array}{l}
\frac{-\beta}{1 + e^{-\frac{m}{2k_F Q^2} \left( \frac{\omega + \hbar k_F Q^2}{2m} \right)^2}} \\
\frac{-\beta}{1 + e^{-\frac{m}{2k_F Q^2} \left( \frac{\omega - \hbar k_F Q^2}{2m} \right)^2}}
\end{array} \right. 
\]

(87)

Corresponding expression for \( v_c^{(r)} \) is found to be

\[ \text{Re} \left( v_c^{(r)}[n,T] \right) = -\hbar k_F \int \frac{d^3 Q}{(2\pi)^3} \int_0^\infty \frac{d\omega}{2\pi} \left( \frac{e^{\beta\hbar \omega} + 1}{e^{\beta\hbar \omega} - 1} \right) \left[ F_1(Q,\omega) + F_2(Q,\omega) + F_3(Q,\omega) \right] \]

(88)
\[ F_1 = \frac{V(Q) (1-V(Q)) \text{Re} \chi(Q,\omega)}{(1-V(Q) \text{Re} \chi(Q,\omega))^2 + (V(Q) \text{Im} \chi(Q,\omega))^2} \]
\[
\times \frac{m^2}{2\pi \hbar^4 \beta k_F Q} \left(\frac{d\alpha}{dn}\right) \left(1 - \frac{1}{\beta \left[ \frac{m}{2k_F Q} \left(\omega + \frac{\beta k_F Q^2}{2m}\right) - \alpha \right] + \alpha} \right) \]
\[
\frac{1}{1 + e} \left(1 - \frac{1}{\beta \left[ \frac{m}{2k_F Q} \left(\omega + \frac{\beta k_F Q^2}{2m}\right) - \alpha \right] + \alpha} \right) \]
\]
\[ F_2 = \frac{V^2(Q) \text{Im} \chi(Q,\omega)}{(1-V(Q) \text{Re} \chi(Q,\omega))^2 + (V(Q) \text{Im} \chi(Q,\omega))^2} \]
\[
\times \frac{m}{2\pi \hbar^2 \beta k_F} \left(\frac{d\alpha}{dn}\right) \int_0^\infty dk \, f(k) \left(1-f(k)\right) \left(\frac{1}{\beta \left[ \frac{m}{2k_F Q} \left(\omega + \frac{\beta k_F Q^2}{2m}\right) - \alpha \right] + \alpha} \right) \]
\[
\times \ln \left| \begin{array}{c}
\omega + \frac{\beta k_F Q^2}{2m} \\
\omega + \frac{\beta k_F Q^2}{2m} \\
\omega - \frac{\beta k_F Q^2}{2m} \\
\omega - \frac{\beta k_F Q^2}{2m}
\end{array} \right|
\]
\[
\times \ln \left| \begin{array}{c}
\frac{\beta k_F Q^2}{m} \\
\frac{\beta k_F Q^2}{m} \\
\frac{\beta k_F Q^2}{m} \\
\frac{\beta k_F Q^2}{m}
\end{array} \right|
\]

and

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
\[ F_3 = -\frac{V(Q) m^2}{2\pi \hbar^4 \beta k_F Q} \left( \frac{d\alpha}{dn} \right) \]

\[
-\left\{ \frac{1}{1 + e^{\beta [\frac{m}{2k_F Q^2} (\omega - \frac{\hbar k_F Q^2}{2m})^2] - \alpha}} \right\}
\]

with \[ \frac{d\alpha}{dn} = \frac{1}{n - \frac{1}{\pi^2} \int_{0}^{\infty} dk k^2 (f(k))^2} \].

However, for the purpose of numerical computation for finite temperatures, it is much more convenient to use the discrete frequency series (82) and (84) rather than the integral version for reasons given below:

(a) Note that the $l = 0$ term of the series alone reproduces the Debye result for $\Omega_c^{(r)}$ and $V_c^{(r)}$ in the $t \to \infty$ limit, where the $Q \to 0$ approximation for the corresponding polarisability is found to be most appropriate. Thus, since
Using (89) in (82), the integral could be carried out analytically to give

\[
\frac{-V(Q) \chi(Q, \ell=0)}{Q \to 0} \xrightarrow{t \to \infty} \left( \frac{4n\pi e^2}{k_B T} \right) \frac{1}{\alpha^2 k_F^2} \tag{89}
\]

the Debye-Hückel result. Similarly, the correlation potential is obtained as

\[
\frac{\Omega_c^{(x)}}{V_0} \xrightarrow{Q \to 0} \frac{2}{3} \sqrt{\pi} \frac{e^{3/2} n^{3/2}}{(k_B T)^{1/2}} \tag{90}
\]

Thus, the \( \ell=0 \) term gives the dominant contribution to both the correlation energy and the potential in the high temperature limit; all other terms vanish faster than (90) or (21). This is expected because in this limit, the divergence at small \( q \) occurs only in the \( \ell=0 \) term.

One can show that, for \( \ell \neq 0 \),

\[
V(q) \chi(q, \frac{2\pi \ell k_B T}{\hbar}) \xrightarrow{t \to \infty} \frac{4\pi e^2 \hbar^2 n}{m(2\pi \ell k_B T)^2}
\]

remains bounded as \( q \to 0 \). Thus one can expand the logarithm and obtain
and the sum over \( \ell \) converges.

(b) For large values of \( t \), typically for \( t > 3 \), only a few terms in the \( \ell \)-series contribute significantly.

(c) The computation of \( \chi(Q, \nu_L) \) for \( \ell \neq 0 \) involves no singularities for any finite \( Q \). This is a major advantage because the integral versions for \( \Omega_c^{(r)} \) and \( \nu_c^{(r)} \) involve complicated singularities in the \( Q-\omega \) plane.

(d) In the numerical evaluation of the \( Q \)-integrals in eq. (82) and (83), the upper limit of \( Q \) is chosen to be a suitable \( Q_{\text{max}} \), so that the contributions from beyond this value are negligible. As \( t \) increases, \( Q_{\text{max}} \) increases and the contributions from the intermediate and large \( Q \) values are quite significant. Even at high density, for example \( n = 10^{26} \text{ cm}^{-3} \), the result obtained from the Gell-Mann-Brueckner approximation involving the \( Q \to 0 \) limit at \( t=0 \) accounts for only about 50\% of the full value of the 'ring' sum.

Computed values of \( \Omega_c^{(r)} \) and \( \nu_c^{(r)} \) are listed in the tables (a)-(d) for the density range \( 10^{26}-10^{18} \text{ cm}^{-3} \) as a function of \( t \). In sharp contrast to the exchange
potential, \( V_x \), \( V_c^{(r)} \) is found to increase initially with \( t \), go through a broad minimum and decrease very slowly with increasing \( t \). The minimum of \( V_c^{(r)} \) shifts gradually to lower \( t \)-values as density increases. The correlation enhancement is found to be more pronounced for high densities; for \( n = 10^{26} \text{ cm}^{-3} \), \( \frac{V_{c}^{\text{min}}}{V_c} (t=0) \) is about 5, dropping to 2 for \( n = 10^{18} \text{ cm}^{-3} \). However, the decay rate of \( V_c^{(r)} \) with \( t \) is much smaller at lower densities. A similar trend is shared by \( \Omega_c^{(r)} \).

In the intermediate degeneracy region, \( 0.3 < t < 3.5 \), \( V_c^{(r)} \) is substantially different from both the \( t=0 \) and \( t=\infty \) limits. At \( t=0 \), our results agree quite well with von Barth and Hadin\(^{36} \) in the metallic density region (\( n \sim 10^{-23}-10^{-24} \)) considered by them. The corresponding high temperature result of DeWitt\(^{38} \) for \( \Omega_c^{(r)} \) expressed as a power series in the plasma parameter

\[
\gamma = \frac{\tau}{\lambda_D}, \text{ where } \tau = \frac{\mathcal{H}}{\sqrt{2mk_BT}} \text{ and } \lambda_D = \left(\frac{k_BT}{4\pi ne^2}\right)^{1/2}
\]

serves as a useful check for our results for both \( \Omega_c^{(r)} \) and \( V_c^{(r)} \). Typically, \( V_c^{(r)} \) merges with this Debye result beyond \( t \sim 10 \).

Fig. 9 exhibits the relative importances of exchange and correlation potentials as a function of \( t \) for various densities. \( V_x \) decreases rapidly through the intermediate degeneracy region and so it crosses over to \( V_c^{(r)} \) counterpart at \( t = t_o \) for a given density. This feature of
correlation contribution dominating over the exchange is of increasing importance for all \( t > t_0 \). The locus of \( t_0 \) as a function of \( n \) distinguishing the two regions \( V_C^{(r)} \gtrsim V_X \) and \( \Omega_C^{(r)} \gtrsim \Omega_X \) is given in Fig. 12. From this, it is evident that at smaller densities, correlation is seen to be more important than exchange over practically the entire temperature range. The same general behaviour is found for \( \Omega_X \) and \( \Omega_C^{(r)} \).

A plot of \( V_{XC} \) vs \( t \) for different densities along with a plot of \( V_X \) vs \( t \) in Fig. 10 exhibits the importance of the use of \( V_{XC} \) in comparison with \( V_X \) alone. For high densities and small \( t \) values, \( V_{XC} \) is dominated by \( V_X \) (\( V_X \) is 84% of \( V_{XC} \) for \( n = 10^{24} \text{ cm}^{-3} \) at \( t=0 \)). But for every density, as \( t \) increases, \( V_X \) diminishes in its effects rapidly so that \( V_C^{(r)} \) dominates over a large \( t \) range. Neglect of correlation thus would lead to significant errors in a wide range of \( n-T \) domain. Note that \( V_{XC} \) as a function of \( t \) has a smoother behaviour than either \( V_X \) or \( V_C^{(r)} \) alone. At low \( t \), enhancement of \( V_C^{(r)} \) partially compensates for the decay of \( V_X \). At large \( t \), the very slow decay of \( V_C^{(r)} \) governs the persistence of \( V_{XC} \).

In an actual application of the local density functional scheme at finite temperatures, one needs to consider the entire density profile, varying from very large
value near the nucleus to a much smaller value far away from the nucleus (merging with the background density of the plasma), in thermal equilibrium at a fixed temperature $T$. A calculation of $V_{xc}[n,T = \text{const.}]$ over a wide range of densities is therefore needed.

The result of such a calculation for typical plasma temperatures $T=1, 10$ and 100 eV, for a wide density range of $10^{26}-10^{18}$ cm$^{-3}$ is presented as a plot of $V_{xc}[n,T]$ scaled by the respective zero-temperature value $V_{xc}[n,0]$ as a function of $n$ (Fig. 11). For each of these temperatures, for high densities, the $t$-value is small—this makes the corresponding ratio $V_{xc}[n,T]/V_{xc}[n,0]$ close to unity. Along each curve, as one moves towards the lower densities, the ratio $t$ gets increasingly larger—this results in making $V_{xc}[n,T]$ substantially different from the corresponding zero temperature value. This 'peeling off' shifts to higher densities as temperature increases. In the intermediate portion of each curve, exchange and correlation plays comparable roles whereas the tail portions are dominated by $V_{c}(r)$. In fact, the values of $V_{xc}[n,T]/V_{xc}[n,0]$ for $n = 10^{18}$ cm$^{-3}$ satisfy an approximate $T^{-1/2}$-scaling, as predicted by eq. (91) for $V_{c}(r)(t=\infty)$.

At this point, a comparison with a recent work of Dharma-Wardana and Taylor is in order. Let us first
point out that their scheme of calculating the exchange correlation correction to the chemical potential, \( \mu_{\text{xc}} \) is different from ours. They obtain the correction \( \Delta N \) to the electron density \( N \) from the thermodynamic relation

\[
\left( \frac{\partial \Omega}{\partial \mu} \right)_T = -N \quad \text{(92)}
\]

The corrected chemical potential is then obtained from

\[
3 \int_0^\infty dx \, x^2 \frac{1}{1 + \frac{e^{(\frac{1}{2}x^2 - \mu/k_B T)}}{N}} = 1 - \frac{\Delta N}{N} \quad \text{(93)}
\]

Note that in (92) \( \mu \) is that of the free gas value, \( \mu_0 \) and \( \Omega = \Omega_0 + \Omega_{\text{xc}} \) has been calculated by using \( \mu_0 \). \( \mu_{\text{xc}} \) determined this way is a very different quantity compared to our \( V_{\text{xc}} = \frac{\delta \Omega_{\text{xc}}}{\delta n} \), which follows naturally from Mermin's theorem.

In computing \( \Omega_{\text{xc}} \), they have included second order exchange contributions \( \Omega_x^{(2)} \) and \( \Omega_o^{(2)} \) in addition to first order exchange and 'ring' diagram contributions. However, in the actual evaluation of the 'ring' sum, they have used (i) The \( q \to 0 \) form of the static polarisability \( \chi(q, \omega=0) \) and (ii) the 'plasmon-pole' approximation for \( \chi(q, \omega \neq 0) \), (iii) a series form involving the zeta function has been used to simplify the sum for large discrete fre-
quencies. The $q \to 0$ form of $\chi(q,0)$ gives the Debye result at finite temperatures and its use for intermediate $t$ values, as they have done, leads to an overestimate of correlation contribution. The plasmon-pole approximation is known to slightly overestimate the R.P.A. energy at $0^\circ$ K; but is of unknown accuracy at arbitrary temperatures. The combined effect of (i) and (ii) is expected to lead to significant overestimate of correlation contribution, particularly at small and intermediate $t$ values, where both the dynamic and the static contributions are important. Lacking details, we shall not comment on approximation (iii). In our evaluation of the 'ring' sum, no approximation at all has been made, either to $q$-dependence or $\omega$-dependence.

Contributions due to $\Omega_x^{(2)}$ and $\Omega_o^{(2)}$, being second order effects are of course much smaller than the first order exchange contribution $\Omega_x^{(1)}$. In addition, $\Omega_x^{(1)} \sim \frac{1}{t}$; whereas $\Omega_o^{(2)} \sim \frac{1}{t^{3/2}}$ for large $t$, as shown in Appendix B. Thus, with increasing temperatures, these contributions vanish faster than even the first order exchange. (In Dharmawardana et al.'s evaluation of $\Omega_x^{(2)}$ and $\Omega_o^{(2)}$, further approximations have been made: static screening has been considered in the $q \to 0$ form, for example).

It is clear from the above discussion that no quantitative comparison could be made with the $\mu_{xc}$ of Ref. 40.
and our $V_{xc}$. However, in their method of evaluating $\mu_{xc}$, it turns out that the linear Hartree-Fock correction to chemical potential coincides with our $V_x$. Here the numerical results between the two computations agree to within 2% or better. For small $t$ range, the agreement is better than 1%. (Values for small $t$ were provided in private communication by Dr. Dharmawardana).

The exchange-correlation potential $V_{xc}$ presented here represents an important step towards a complete development of the density functional scheme for inhomogeneous electron systems at finite temperature. The most important results that emerge from our investigation are (i) in contrast to $\Omega_x$ and $V_x$, the correlation free energy $\Omega_c^{(r)}$ and potential $V_c^{(r)}$ are enhanced initially for low temperatures and (ii) the persistence of correlation effects at high temperature—so that for a wide range of densities and temperatures, correlation effects are more important than exchange effects.

The exchange-correlation potential $V_{xc}[n,T]$ developed here represents an important step in the systematic development of the local density functional scheme at finite temperatures. In the following chapter, we consider an application of $V_{xc}$ to study the spectrum of a neon impurity in a dense, hot laser plasma.
CHAPTER V

THE EXCHANGE-CORRELATION POTENTIAL:
AN APPLICATION

In the Hartree scheme, all exchange-correlation effects are neglected. The purpose of the following calculation is to study the effect of on the Kohn-Sham eigenvalues $\varepsilon_i$'s when the appropriate $V_{xc}[n,T]$ is included in the calculation.

Consider a neon nucleus ($Z=10$) embedded in a plasma of electron density $n = 10^{24}$ electrons/cm$^3$ at a temperature $T = 100$ eV = $1.2 \times 10^6$ K, as in a typical laser-imploded plasma. The calculations are done in two stages:

(1) All exchange-correlation effects are neglected as a first approximation. In that case, the effective single particle potential is

$$ V_{\text{eff}}^i = -\frac{Ze^2}{r} + e^2 \int \frac{n(r',T) \, dr'}{|r-r'|} $$

with $n(r,T)$ determined from

$$ n(r,T) = \sum_i |\psi_i(r)|^2 / \left[ e^{(\varepsilon_i - \mu)/kT} + 1 \right] ,$$

where the sum is over all occupied states, both bound and continuum. The $\{\varepsilon_i, \psi_i(r)\}$ are obtained by solving the single-particle equation:
Equations (94) to (96) were solved self-consistently by D. A. Liberman (Los Alamos National Laboratory) to obtain the 1s, 2s, 2p eigenvalues for neon. The results are given in Table 13.

In the second stage, the self-consistent charge densities \( n(\hat{r}, T) \) obtained in the above calculation was used to construct a new effective potential \( V_{\text{eff}}^{\text{II}} \), which includes the appropriate \( V_{\text{xc}}[n(\hat{r}), T] \) associated with the self-consistent charge density profile \( n(\hat{r}, T) \), i.e.,

\[
V_{\text{eff}}^{\text{II}} = V_{\text{eff}}^{\text{I}} + V_{\text{xc}}[n(\hat{r}), T = 100 \text{ eV}]
\]

The single-particle equation (96) was then solved using \( V_{\text{eff}}^{\text{II}} \) by Numerov method to obtain the new 1s, 2s, and 2p eigenvalues.

As seen from Table 13, the effect of including \( V_{\text{xc}}[n(\hat{r}), T] \) on the bound state spectrum is found to be very substantial. \( \epsilon_{1s} \) is lowered by about 6%, \( \epsilon_{2s} \) by 20% and \( \epsilon_{2p} \) by as much as 30% compared to the self-consistent Hartree result.

The result is best understood by referring to the schematic diagram of Fig. 13. The charge density profile \( n(\hat{r}, T = 100 \text{ eV}) \) obtained from self-consistent Hartree scheme peaks to about \( 10^{28} \) electrons/cm\(^3\) \( (t = 0.006) \) at
the position of the nucleus (the origin), drops rapidly through the intermediate r-region and merges slowly to the surrounding plasma density of $10^{24}$ electrons/cm$^3$ $(t = 2.74)$ beyond $r = 2.1 a_0$. The corresponding self-consistent potential $V_{\text{eff}}^I$ (curve I) thus rapidly weakens in the intermediate r-range and vanishes for $r \geq 2.1 a_0$.

$V_{\text{eff}}^{II} = V_{\text{eff}}^I + V_{xc} [n(r), T = 100 \text{ ev}]$ is practically indistinguishable from $V_{\text{eff}}^I$ in the small r-range since $V_{xc}$ is very small compared to $V_{\text{eff}}^I$. In the large r-range, the Hartree term nearly cancels out the nuclear term. Thus $V_{xc}$ governs the behaviour of $V_{\text{eff}}^{II}$ in this range, making it substantially deeper than $V_{\text{eff}}^I$. The energy level spectrum supported by $V_{\text{eff}}^{II}$ is thus significantly deeper than that due to $V_{\text{eff}}^I$ -- the effect being much larger on the higher lying states (Table 13).

In the actual computation, the exchange correlation potential $V_{xc} [n_0, T]$ corresponding to the uniform background density of $10^{24}$ electrons/cm$^3$ is subtracted from $V_{\text{eff}}^{II}$, so that $\tilde{V}(r) = V_{\text{eff}}^{II}(r) - V_{xc} [n_0, T]$ vanishes for large r. This is needed for solving the Schrödinger equation by Numerov method since the condition that the wave function vanishes for large r could be incorporated. The eigenvalues $\tilde{\epsilon}_i$'s obtained by using $\tilde{V}$ are, of course, related to the usual eigenvalues $\epsilon_i$'s as

$$\tilde{\epsilon}_i = \epsilon_i + V_{xc} [n_0, T]$$
This calculation clearly illustrates that the effect of the exchange-correlation potential could be very substantial on the Kohn-Sham eigenvalues $\varepsilon_i$'s which is missed in a Hartree scheme. The use of $V_{xc}[n,T]$ lowers the eigenvalues and the corresponding occupation probabilities are thereby increased (Table 13). This, in turn, affects the grand potential $\Omega[n,T]$ as given by equation (18e) and consequently all the thermodynamic properties.

Also, as seen from Table 13, the use of $V_{xc}$ reduces the line shift $\Delta E_{1s-2p}$ substantially. Since the transition probability is proportional to $(\Delta E_{1s-2p})^3$, the intensity of the emitted line is affected drastically. This has its importance for plasma diagnostics.

A full self-consistent calculation required the development of a huge computer program to solve the finite temperature Kohn-Sham equations iteratively. In addition to the bound state, the continuum states have to be handled via the phase shift calculations. The use of the exchange correlation potential $V_{xc}[n,T]$ developed in previous chapters in such a self-consistent calculation is of primary interest.

Such a calculation has recently been done by Perrot to study the problem of a proton embedded in a dense, hot electron plasma. In his calculation, he used an analytical fit to our $V_{xc}[n,T]$ to carry out the computation. Because of the relevance of
the work, some of his results are presented in Table 14. The displaced electron density $n$ at the proton site obtained by self-consistent L.D.A. is compared to the corresponding results obtained from linear screening theory as a function of electron density through the intermediate degeneracy region. The charge pile-ups predicted by L.D.A. is substantially larger than those obtained from linear screening. However, the differences are reduced with increasing density—indicating that the linear screening scheme gets better as density increases. Also, for every density, the linear screening results are closer to the self-consistent results at higher temperatures than at zero temperatures. This is expected, since the charge distribution is smeared out with increased temperatures.

The Kohn-Sham eigenvalues in the finite temperature L.D.A. calculation are lowered with increasing temperatures—a trend shared by linear screening theory. Also, as discussed by Perrot, the extra energy associated with the impurity, $\Delta E$, calculated according to the finite temperature L.D.A. scheme are quite comparable to the linear TF-screening results.
CHAPTER VI
SUMMARY AND CONCLUDING REMARKS

Let us now summarize the major aspects of the present work. The density and temperature dependent exchange-correlation potential $V_{\text{xc}}[n,T]$ developed here represents an important step in the systematic generalization of the local density functional theory to finite temperatures. As emphasized before, our exchange-correlation potential is consistent with Mermin's theorem and is the appropriate one to use in a self-consistent scheme to obtain the equilibrium properties of physical systems at finite temperatures. For purpose of rapid computation a fitted form of our $V_{\text{xc}}[n,T]$ is very useful.

From our analysis, the correlation effects are found to play a very important role at high temperatures. The fact that the correlation potential $V_{\text{c}}^{(r)}[n,T]$ (as also $\Omega_{\text{c}}^{(r)}[n,T]$) is enhanced above the zero temperature value for small $t$ and decays very slowly as temperature increases is a striking result that emerges from our investigation and is extremely important for high temperature plasmas. Firstly, this enhancement largely compensates the decay of exchange effect for small and intermediate $t$ region—as a result $V_{\text{xc}}[n,T]$ is much larger in magnitude than what one obtains by considering exchange effect alone. Secondly, as $t$ increases, the relative importance of correlation effect increases; at very high temperatures, $V_{\text{xc}}$ as well as $\Omega_{\text{xc}}$ is completely dominated.
by correlation effects. The persistence of correlation effects at high temperatures is important both for equation of state calculations as well as in determining atomic properties of charged impurities used as diagnostic tools in plasmas.

As pointed out in Chapter IV, the exchange-correlation energy and potentials have been obtained by a perturbation method and therefore, is valid for the 'weakly coupled' plasma conditions. For 'strongly-coupled' regime, i.e., for low densities and low temperatures, the potential energy can no longer be treated as a small perturbation to the kinetic energy term. A non-perturbative treatment of electron interaction is thus called for. The schemes of Totsuji and Ichimaru\(^{41}\) (TI) and of Vashita and Singwi\(^{42}\) (VS) deserve special attention in this context.

In the TI-scheme, the approach is via the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) equations for a classical system of \(n\) identical particles. The integro-differential equation for one particle distribution function \(f(1)\) involves the two-particle correlation function \(f(12)\). The two-particle correlation function described by the second BBGKY equation, in turn, involves the three-particle correlation function \(f(123)\) and so on. The ansatz used in TI-schemes are:

\[
 f(12) = f(1) f(2) g(|\vec{r}_1 - \vec{r}_2|)
\]

and

\[
 f(123) = f(1) f(2) f(3) h(|\vec{r}_1 - \vec{r}_2|, |\vec{r}_2 - \vec{r}_3|, |\vec{r}_3 - \vec{r}_1|)
\]
with
\[ h(|\vec{r}_1-\vec{r}_2|,|\vec{r}_2-\vec{r}_3|,|\vec{r}_3-\vec{r}_1|) = g(|\vec{r}_1-\vec{r}_2|) \ g(|\vec{r}_2-\vec{r}_3|) \]
\[ + \ g(|\vec{r}_2-\vec{r}_3|) \ g(|\vec{r}_3-\vec{r}_1|) + g(|\vec{r}_3-\vec{r}_1|) \ g(|\vec{r}_1-\vec{r}_2|) \]
\[ + \int d\vec{r}_4 \ g(|\vec{r}_1-\vec{r}_4|) \ g(|\vec{r}_2-\vec{r}_4|) \ g(|\vec{r}_3-\vec{r}_4|) \],
where \( g(|\vec{r}_1-\vec{r}_2|) \) is the pair-correlation function of two particles located at \( \vec{r}_1 \) and \( \vec{r}_2 \) and \( h \) is the ternary correlation function. These ansatzes are used in the first and second BBGKY equations. The fourier transform of these equations lead to the following integral equations for the static structure factor \( S(k) \):
\[ S(k) - 1 = -\frac{k^2}{k^2 + k_D^2} t(k) \ \{ t(k) + S(k) [\omega(k) - u(k)] \} \]
where
\[ t(k) = 1 + u(k) = 1 + \frac{1}{n} \sum \limits_{q} \frac{k \cdot q}{q^2} [S(|k-q|) - 1] \]
\[ \omega(k) = \frac{1}{n} \sum \limits_{q} \frac{k \cdot q}{q^2} S(q) [S(|k-q|) - 1] \],
and
\[ k_D^2 = 4\pi n e^2/(k_B T) \].
These equations are solved self-consistently on a computer for \( S(k) \). The correlation energy \( E_C \) is then obtained as
\[ \frac{E_C}{n k_B T} = \Gamma \int_{0}^{\infty} \frac{dk}{k_D} [S(k) - 1] \].
\[ \Gamma = (4\pi n)^{1/2} e^3 (k_B T)^{-3/2} \], is the usual plasma coupling parameter).

Let us note that in the scheme, three-particle correlations have been included in an approximate way along with the two-particle correlation. This is an improvement over the finite temperature R.P.A. ('ring' approximation) scheme which does not include any three-particle correlation. In addition, the self-consistent determination of the static structure factor \( S(k) \) goes beyond a perturbation scheme. These improvements are reflected in the fact that the correlation energy \( E_c \) obtained from the TI-scheme are in excellent agreement with the elaborate Monte-Carlo calculation of Brush, Sahlin and Teller\(^{44} \) in the moderately strong-coupling region: \( 1 < \Gamma < 10 \).

The Vashista-Singwi (VS) scheme, developed to treat electron-correlations at zero temperature, may be considered as the quantum mechanical analog of the TI-scheme. Once again, three-particle correlations are included in an approximate way via the density deviative of the equilibrium pair correlation function. As a result, the wave-vector and frequency dependent dielectric function \( \varepsilon(q,\omega) \) for electrons of density \( n \) is modified by a 'local field correction' \( G(q) \):

\[
\varepsilon(q,\omega) = 1 + \frac{V(q) \chi(q,\omega)}{1 - G(q) V(q) \chi(q,\omega)} ; \quad V(q) = \frac{4\pi e^2}{q^2}
\]
with
\[
G(q) = \left( 1 + \frac{n}{2} \frac{\partial}{\partial n} \right) \left( -\frac{1}{n} \int \frac{dq}{(2\pi)^3} \frac{q}{q'Z} \left[ S(q-q') - 1 \right] \right)
\]

(\chi(q,\omega) is the usual Lindhard polarisability.) The static structure factor \( S(q) \), on the other hand, is related to \( \varepsilon(q,\omega) \) back again via the fluctuation-dissipation theorem:
\[
S(q) = -\frac{\hbar q^2}{4\pi ne^2} \int_0^\infty d\omega \text{Im} \left[ \frac{1}{\varepsilon(q,\omega)} \right]
\]

The above three equations again constitute a self-consistent scheme to calculate \( S(q) \). In their numerical evaluation, VS have used the Hartree-Fock structure factor as the starting input for the iteration scheme. The self-consistent \( S(q) \) is then used to calculate the correlation energy \( \varepsilon_c \) for the electron liquid at zero temperature.

Note that without the 'local field correction' \( G(q) \), the VS \( \varepsilon(q,\omega) \) would have reduced to the usual zero temperature R.P.A. result. The self-consistent scheme of determining the structure factor, and hence the correlation energy, of course, goes beyond a perturbation treatment.

In the metallic density region (intermediate coupling regime), this non-perturbation method naturally yields better results for the correlation energies. Further, the pair-correlation function \( g(r) \), which show the unphysical behaviour of becoming negative for small \( r \) within the R.P.A., is also improved substantially.
For the strong coupling regime, therefore, the TI and the VS schemes are suitable for dealing with electron correlation effects. As already noted, the VS-scheme was developed for $T=0$, although a calculation for small temperatures has recently been reported. The generalization of the VS-scheme to arbitrary temperatures is of major interest. In particular, we suggest the use of the finite temperature Hartree-Fock structure factor as a starting input for the self-consistent determination of $S(q,T)$ needed to calculate $\Omega_C[n,T]$. A further improvement would be to include the dynamic ($\omega$) dependence of the local field factor $G$, which may be significant for finite temperatures. Once $\Omega_C[n,T]$ is obtained, the correlation potential $V_C[n,T]$ appropriate for strongly coupled plasmas could be extracted in the usual way. This potential would then supplement our $V_{xc}[n,T]$ appropriate for the weakly coupled plasmas. Within the scheme, the exchange-correlation potential we have is the most complete one of its kind so far. Also, this $V_{xc}[n,T]$ is to be used as inputs in a self-consistent scheme. As in the case with zero temperature Kohn-Sham equations, the self-consistent scheme does improve the situation still further.

We have pointed out the connection between the Kohn-Sham effective potential and the screened impurity potential at finite temperatures. The generalization of the R.P.A.-screened potential to finite temperatures gives us
a very useful scheme that interpolates naturally between the well-known Thomas-Fermi screening in the degenerate level and the Debye screening in the classical limit. Within the scheme, complete analysis of full momentum dependence and degeneracy effect have been done. Useful estimates of line shifts, breaking of Coulomb degeneracy etc., could be obtained from this. In addition, the phase shifts and the energy levels one obtains from the screened potential could be used to calculate the interacting part of the partition function and in a variety of plasma calculations. Comparison with other screening models and self-consistent calculations by Skupsky\textsuperscript{11} and Perrot\textsuperscript{12} shows that our model tends to get better with increasing density and higher temperatures. However, in the actual plasma conditions, the static screened potential is not adequate. Even in the case of an ion, the bound electrons will relate to a frequency component of the field associated with the level frequency and not necessarily to a static potential. A fully dynamic screened potential, valid for arbitrary degeneracies—is thus required. Such a dynamic screened potential arises naturally in a many-body approach to the problem. The scheme has been outlined by Majumdar\textsuperscript{46} and by Rajagopal\textsuperscript{47}, et al. for electron-positron bound states in a many-body system. The positive and negative charges are treated on an equal footing; and finite temperature
Green's function-approach leads to an effective equation governing the two-particle energy spectrum in a many-body system as for partially ionized atoms in a hot, dense plasma. Shifted energy levels and finite lifetimes due to the effect of the surrounding plasma arises naturally in this theory. It can be shown\textsuperscript{48} that in the non-degenerate limit, the effective two-particle equation coincides in the center-of-mass frame, with the Schrödinger equation for a charged particle moving in a static-screened Debye potential, which was treated in Chapter II.

A full execution of the many-body scheme is a formidable task due to the extreme complexity of the problem. Some preliminary work in this direction has been done by Zimmerman\textsuperscript{49}, et al. as well as the Dharma-Wardana\textsuperscript{45}, et al. A full implementation of the scheme is, however, far from being complete and in view of the importance of the problem in plasma physics it remains as a major task for the future.
REFERENCES


Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.


<table>
<thead>
<tr>
<th>Electron Densities (cm(^{-3}))</th>
<th>Fermi Temperature (T_F(\text{^0K}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(10^{18})</td>
<td>42.3</td>
</tr>
<tr>
<td>(10^{20})</td>
<td>911.3</td>
</tr>
<tr>
<td>(10^{22})</td>
<td>(2 \times 10^4)</td>
</tr>
<tr>
<td>(10^{24})</td>
<td>(4.2 \times 10^5)</td>
</tr>
<tr>
<td>(10^{26})</td>
<td>(9.1 \times 10^6)</td>
</tr>
<tr>
<td>(10^{28})</td>
<td>(2 \times 10^8)</td>
</tr>
</tbody>
</table>
### TABLE 1b

<table>
<thead>
<tr>
<th>Physical Systems</th>
<th>Typical Electron Densities (cm^-3)</th>
<th>Typical Temperatures</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laboratory plasmas</td>
<td>(10^{11} - 10^{16})</td>
<td>arbitrary</td>
</tr>
<tr>
<td>Highly doped semiconductors</td>
<td>(10^{17} - 10^{19})</td>
<td>(3 \times 10^2)</td>
</tr>
<tr>
<td>Metals</td>
<td>(10^{21} - 10^{23})</td>
<td>(3 \times 10^2)</td>
</tr>
<tr>
<td>Dense laser-plasmas</td>
<td>(10^{21} - 10^{24})</td>
<td>(10^4 - 10^8)</td>
</tr>
<tr>
<td>Shock-compressed solids</td>
<td>(10^{24} - 10^{25})</td>
<td>(10^4 - 10^5)</td>
</tr>
<tr>
<td>Stellar interior</td>
<td>(10^{26})</td>
<td>(\sim 10^7)</td>
</tr>
</tbody>
</table>
| White dwarf               | \(10^{28}\)                      | \(10^4 - 10^7\)      | (estimated)
<table>
<thead>
<tr>
<th>$t$</th>
<th>$\zeta^2(Q=0,n,t)/\zeta_{TF}^2$ (eq. (33))</th>
<th>$\alpha \Xi \mu / k_B T$ (eq. (30))</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.9918</td>
<td>9.9180</td>
</tr>
<tr>
<td>0.2</td>
<td>0.9614</td>
<td>4.8229</td>
</tr>
<tr>
<td>0.4</td>
<td>0.8447</td>
<td>2.1009</td>
</tr>
<tr>
<td>0.6</td>
<td>0.7183</td>
<td>1.0415</td>
</tr>
<tr>
<td>1.0</td>
<td>0.5292</td>
<td>-0.0214</td>
</tr>
<tr>
<td>1.5</td>
<td>0.3890</td>
<td>-0.7489</td>
</tr>
<tr>
<td>2.0</td>
<td>0.3051</td>
<td>-1.2307</td>
</tr>
<tr>
<td>2.5</td>
<td>0.2501</td>
<td>-1.5920</td>
</tr>
<tr>
<td>3.0</td>
<td>0.2116</td>
<td>-1.8815</td>
</tr>
<tr>
<td>3.5</td>
<td>0.1832</td>
<td>-2.1233</td>
</tr>
</tbody>
</table>

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
<table>
<thead>
<tr>
<th>Plasma Density (cm⁻³)</th>
<th>t = t / t_f</th>
<th>( E (\text{Ryd}) ) using Debye potential</th>
<th>( E (\text{Ryd}) ) using effective potential</th>
<th>% lower than Debye (combined T and Q effects)</th>
<th>( E (\text{Ryd}) ) using temperature-dependent Thomas-Fermi potential</th>
<th>% lower than Debye (T effect only)</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.67 × 10²²</td>
<td>2.00</td>
<td>-0.397</td>
<td>-0.495</td>
<td>22</td>
<td>-0.485</td>
<td>-0.485</td>
</tr>
<tr>
<td>6.8 × 10²¹</td>
<td>1.02</td>
<td>-0.255</td>
<td>-0.365</td>
<td>59</td>
<td>-0.365</td>
<td>-0.365</td>
</tr>
<tr>
<td>2.6 × 10²²</td>
<td>0.66</td>
<td>-0.182</td>
<td>-0.413</td>
<td>0.60</td>
<td>-0.413</td>
<td>-0.413</td>
</tr>
<tr>
<td>1.8 × 10²¹</td>
<td>0.60</td>
<td>-0.131</td>
<td>-0.365</td>
<td>1.02</td>
<td>-0.365</td>
<td>-0.365</td>
</tr>
<tr>
<td>1.4 × 10²¹</td>
<td>0.131</td>
<td>-0.255</td>
<td>-0.413</td>
<td>1.02</td>
<td>-0.413</td>
<td>-0.413</td>
</tr>
<tr>
<td>1.0 × 10²¹</td>
<td>0.131</td>
<td>-0.255</td>
<td>-0.413</td>
<td>1.02</td>
<td>-0.413</td>
<td>-0.413</td>
</tr>
<tr>
<td>0.6 × 10²¹</td>
<td>0.131</td>
<td>-0.255</td>
<td>-0.413</td>
<td>1.02</td>
<td>-0.413</td>
<td>-0.413</td>
</tr>
<tr>
<td>0.5 × 10²¹</td>
<td>0.131</td>
<td>-0.255</td>
<td>-0.413</td>
<td>1.02</td>
<td>-0.413</td>
<td>-0.413</td>
</tr>
<tr>
<td>0.2 × 10²¹</td>
<td>0.131</td>
<td>-0.255</td>
<td>-0.413</td>
<td>1.02</td>
<td>-0.413</td>
<td>-0.413</td>
</tr>
<tr>
<td>0.1 × 10²¹</td>
<td>0.131</td>
<td>-0.255</td>
<td>-0.413</td>
<td>1.02</td>
<td>-0.413</td>
<td>-0.413</td>
</tr>
<tr>
<td>0.05 × 10²¹</td>
<td>0.131</td>
<td>-0.255</td>
<td>-0.413</td>
<td>1.02</td>
<td>-0.413</td>
<td>-0.413</td>
</tr>
<tr>
<td>0.025 × 10²¹</td>
<td>0.131</td>
<td>-0.255</td>
<td>-0.413</td>
<td>1.02</td>
<td>-0.413</td>
<td>-0.413</td>
</tr>
<tr>
<td>0.0125 × 10²¹</td>
<td>0.131</td>
<td>-0.255</td>
<td>-0.413</td>
<td>1.02</td>
<td>-0.413</td>
<td>-0.413</td>
</tr>
<tr>
<td>0.00625 × 10²¹</td>
<td>0.131</td>
<td>-0.255</td>
<td>-0.413</td>
<td>1.02</td>
<td>-0.413</td>
<td>-0.413</td>
</tr>
<tr>
<td>0.003125 × 10²¹</td>
<td>0.131</td>
<td>-0.255</td>
<td>-0.413</td>
<td>1.02</td>
<td>-0.413</td>
<td>-0.413</td>
</tr>
<tr>
<td>0.0015625 × 10²¹</td>
<td>0.131</td>
<td>-0.255</td>
<td>-0.413</td>
<td>1.02</td>
<td>-0.413</td>
<td>-0.413</td>
</tr>
<tr>
<td>0.00078125 × 10²¹</td>
<td>0.131</td>
<td>-0.255</td>
<td>-0.413</td>
<td>1.02</td>
<td>-0.413</td>
<td>-0.413</td>
</tr>
<tr>
<td>0.000390625 × 10²¹</td>
<td>0.131</td>
<td>-0.255</td>
<td>-0.413</td>
<td>1.02</td>
<td>-0.413</td>
<td>-0.413</td>
</tr>
<tr>
<td>0.0001953125 × 10²¹</td>
<td>0.131</td>
<td>-0.255</td>
<td>-0.413</td>
<td>1.02</td>
<td>-0.413</td>
<td>-0.413</td>
</tr>
<tr>
<td>Plasma Density (cm$^{-3}$)</td>
<td>Potential Used</td>
<td>Bound States</td>
<td></td>
<td></td>
<td></td>
<td>Line Shift</td>
</tr>
<tr>
<td>---------------------------</td>
<td>----------------</td>
<td>--------------</td>
<td>--------------</td>
<td>-------</td>
<td>-----</td>
<td>----------</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1s</td>
<td>2s</td>
<td>2p</td>
<td>$\Delta E_{2s-2p}$</td>
<td>$\Delta E_{1s-2p}$</td>
</tr>
<tr>
<td>$4.54 \times 10^{24}$ (t = 1)</td>
<td>$V_D$</td>
<td>-72.816</td>
<td>-5.316</td>
<td>-4.076</td>
<td>1.240</td>
<td>68.740</td>
</tr>
<tr>
<td></td>
<td>$V_\xi$</td>
<td>-75.499 (3.7%)</td>
<td>-6.623 (24.6%)</td>
<td>-5.560</td>
<td>1.063</td>
<td>69.939</td>
</tr>
<tr>
<td></td>
<td>$V_{\text{eff}}$</td>
<td>-78.695 (8.1%)</td>
<td>-7.383 (38.9%)</td>
<td>-6.591</td>
<td>0.792</td>
<td>72.104</td>
</tr>
<tr>
<td>$2.47 \times 10^{24}$ (t = 1.5)</td>
<td>$V_D$</td>
<td>-79.369</td>
<td>-8.747</td>
<td>-7.939</td>
<td>0.808</td>
<td>71.430</td>
</tr>
<tr>
<td></td>
<td>$V_\xi$</td>
<td>-80.605 (1.6%)</td>
<td>-9.487 (8.5%)</td>
<td>-8.759</td>
<td>0.728</td>
<td>71.846</td>
</tr>
<tr>
<td></td>
<td>$V_{\text{eff}}$</td>
<td>-82.800 (4.3%)</td>
<td>-9.930 (13.5%)</td>
<td>-9.330</td>
<td>0.600</td>
<td>73.470</td>
</tr>
<tr>
<td>$1.0 \times 10^{24}$ (t = 2.74)</td>
<td>$V_D$</td>
<td>-86.842</td>
<td>-13.406</td>
<td>-13.022</td>
<td>0.384</td>
<td>73.460</td>
</tr>
<tr>
<td></td>
<td>$V_\xi$</td>
<td>-86.842 (0.4%)</td>
<td>-13.668 (2%)</td>
<td>-13.302</td>
<td>0.366</td>
<td>73.540</td>
</tr>
<tr>
<td></td>
<td>$V_{\text{eff}}$</td>
<td>-88.043 (1.8%)</td>
<td>-14.037 (4.7%)</td>
<td>-13.781</td>
<td>0.256</td>
<td>74.262</td>
</tr>
<tr>
<td>Plasma Density (cm(^{-3}))</td>
<td>Bound States</td>
<td>(\Delta E_{1s-2p} )</td>
<td>(\Delta E_{2s-2p} )</td>
<td>Line Shift</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-----------------------------</td>
<td>--------------</td>
<td>------------------</td>
<td>------------------</td>
<td>------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( t = 7.50 ) ( \times 10^{24} )</td>
<td>4.54</td>
<td>-89.363</td>
<td>-15.564</td>
<td>0.245</td>
<td>74.044</td>
<td>0.356</td>
</tr>
<tr>
<td>( t = 11.25 ) ( \times 10^{24} )</td>
<td>2.47</td>
<td>-89.718</td>
<td>-15.710</td>
<td>0.266</td>
<td>74.234</td>
<td>0.766</td>
</tr>
<tr>
<td>( t = 20.55 ) ( \times 10^{24} )</td>
<td>1.04</td>
<td>-92.068</td>
<td>-17.603</td>
<td>0.141</td>
<td>74.465</td>
<td>0.535</td>
</tr>
</tbody>
</table>

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
<table>
<thead>
<tr>
<th>Plasma Density (10^24 cm⁻³)</th>
<th>V_eff</th>
<th>Linear Debye-Hückel</th>
<th>Vp_Skupsky</th>
<th>Vp from Skupsky</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.54</td>
<td>0.77</td>
<td>0.75</td>
<td>0.68</td>
<td>0.81</td>
</tr>
<tr>
<td>2.47</td>
<td>0.43</td>
<td>0.31</td>
<td>0.38</td>
<td>0.43</td>
</tr>
<tr>
<td>1.00</td>
<td>0.16</td>
<td>0.10</td>
<td>0.15</td>
<td>0.17</td>
</tr>
</tbody>
</table>

TABLE 5a

NEON LYMAN-α LINE SHIFTS (T=750 eV)
TABLE 5b

NEON SPECTRUM: BREAKING OF COULOMB DEGENERACY $\Delta E_{2s-2p}$ (T=750 eV)

<table>
<thead>
<tr>
<th>Plasma Density $\left(10^{24} \text{ cm}^{-3}\right)$</th>
<th>$V_{\text{eff}}$</th>
<th>Skupsky</th>
<th>Linear Debye-Hückel</th>
<th>$V_D$</th>
<th>$V_{\text{SP}}$ (from Skupsky)</th>
<th>$V_{\text{IS}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.54</td>
<td>0.23</td>
<td>0.27</td>
<td>0.61</td>
<td>0.25</td>
<td>0.37</td>
<td>0.36</td>
</tr>
<tr>
<td>2.47</td>
<td>0.13</td>
<td>0.08</td>
<td>0.33</td>
<td>0.14</td>
<td>0.18</td>
<td>0.16</td>
</tr>
<tr>
<td>1.00</td>
<td>0.05</td>
<td>0.03</td>
<td>0.13</td>
<td>0.06</td>
<td>0.07</td>
<td>0.08</td>
</tr>
<tr>
<td>Plasma Density (x 10^24 cm^-3)</td>
<td>Bound States 1s</td>
<td>Bound States 2s</td>
<td>Line Shift ΔE_{ls-2p}</td>
<td>Line Shift ΔE_{2s-2p}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>--------------------------------</td>
<td>----------------</td>
<td>----------------</td>
<td>------------------------</td>
<td>------------------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.1</td>
<td>-94.860</td>
<td>-19.879</td>
<td>0.007</td>
<td>74.981</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.5</td>
<td>-91.219</td>
<td>-16.305</td>
<td>0.036</td>
<td>74.914</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td>-88.944</td>
<td>-14.115</td>
<td>0.076</td>
<td>74.829</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.0</td>
<td>-86.084</td>
<td>-11.430</td>
<td>0.152</td>
<td>74.654</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.0</td>
<td>-81.156</td>
<td>-7.059</td>
<td>0.398</td>
<td>74.097</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.0</td>
<td>-76.328</td>
<td>-3.309</td>
<td>0.832</td>
<td>73.019</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
### TABLE 7

<table>
<thead>
<tr>
<th>Electron Density ( n(\text{cm}^{-3}) \times 10^{18} )</th>
<th>( T = 300^\circ \text{K} ) (All units in rydbergs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Potential Used</td>
<td>1s</td>
</tr>
<tr>
<td>( V_D )</td>
<td>4.776</td>
</tr>
<tr>
<td>( V_5 )</td>
<td>6.674</td>
</tr>
<tr>
<td>( t = 2.5 )</td>
<td>( t = 0 )</td>
</tr>
<tr>
<td>( V_D )</td>
<td>10.275</td>
</tr>
</tbody>
</table>

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
### TABLE 8

**SINGLY CHARGED DONOR IMPURITY IN SILICON (K = 11.8)**

**AT ROOM TEMPERATURE (T = 300° K), UNIT OF ENERGY = ε²/(2a₀ K²)**

<table>
<thead>
<tr>
<th>Carrier Concentration (cm⁻³)</th>
<th>Potential Used</th>
<th>1s</th>
<th>2s</th>
<th>2p</th>
<th>ΔE₁s-2p</th>
<th>ΔE₂s-2p</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2.36 \times 10^{18})</td>
<td>(V_{TF})</td>
<td>0.2340</td>
<td>x</td>
<td>x</td>
<td></td>
<td></td>
</tr>
<tr>
<td>((t = 4.0))</td>
<td>(V_ξ)</td>
<td>0.6101</td>
<td>0.0124</td>
<td>x</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(V_{eff})</td>
<td>0.7094</td>
<td>0.0174</td>
<td>x</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(1.98 \times 10^{18})</td>
<td>(V_{TF})</td>
<td>0.2476</td>
<td>x</td>
<td>x</td>
<td></td>
<td></td>
</tr>
<tr>
<td>((t = 4.5))</td>
<td>(V_ξ)</td>
<td>0.6374</td>
<td>0.0194</td>
<td>0.0032</td>
<td>0.6342</td>
<td>0.0162</td>
</tr>
<tr>
<td></td>
<td>(V_{eff})</td>
<td>0.7279</td>
<td>0.0252</td>
<td>0.0061</td>
<td>0.7218</td>
<td>0.0191</td>
</tr>
<tr>
<td>(1.69 \times 10^{18})</td>
<td>(V_{TF})</td>
<td>0.2597</td>
<td>x</td>
<td>x</td>
<td></td>
<td></td>
</tr>
<tr>
<td>((t = 5.0))</td>
<td>(V_ξ)</td>
<td>0.6606</td>
<td>0.0265</td>
<td>0.0106</td>
<td>0.6500</td>
<td>0.0159</td>
</tr>
<tr>
<td></td>
<td>(V_{eff})</td>
<td>0.7442</td>
<td>0.0328</td>
<td>0.0143</td>
<td>0.7299</td>
<td>0.0185</td>
</tr>
<tr>
<td>$t = T/T_f$</td>
<td>$\Omega_x[n,T]$</td>
<td>$v_x[n,T]$</td>
<td>$\Omega_x[n,0]$</td>
<td>$v_x[n,0]$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>---------</td>
<td>-----------------</td>
<td>-----------</td>
<td>-----------------</td>
<td>-----------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.1</td>
<td>0.959</td>
<td>0.991</td>
<td>0.959</td>
<td>0.991</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.2</td>
<td>0.868</td>
<td>0.967</td>
<td>0.868</td>
<td>0.967</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.3</td>
<td>0.775</td>
<td>0.925</td>
<td>0.775</td>
<td>0.925</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.4</td>
<td>0.687</td>
<td>0.853</td>
<td>0.687</td>
<td>0.853</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.6</td>
<td>0.548</td>
<td>0.721</td>
<td>0.548</td>
<td>0.721</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td>0.382</td>
<td>0.532</td>
<td>0.382</td>
<td>0.532</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.5</td>
<td>0.272</td>
<td>0.381</td>
<td>0.272</td>
<td>0.381</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.0</td>
<td>0.210</td>
<td>0.306</td>
<td>0.210</td>
<td>0.306</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.5</td>
<td>0.171</td>
<td>0.251</td>
<td>0.171</td>
<td>0.251</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.0</td>
<td>0.149</td>
<td>0.212</td>
<td>0.149</td>
<td>0.212</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.5</td>
<td>0.128</td>
<td>0.191</td>
<td>0.128</td>
<td>0.191</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.0</td>
<td>0.089</td>
<td>0.133</td>
<td>0.089</td>
<td>0.133</td>
<td></td>
<td></td>
</tr>
<tr>
<td>t</td>
<td>$-\frac{\Omega}{N}$</td>
<td>$-\frac{V_x}{x}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>----</td>
<td>-----------------</td>
<td>-----------------</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.1</td>
<td>3.479</td>
<td>4.794</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.2</td>
<td>3.149</td>
<td>4.67</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.3</td>
<td>2.812</td>
<td>4.475</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.4</td>
<td>2.493</td>
<td>4.126</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.6</td>
<td>1.988</td>
<td>3.488</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td>1.386</td>
<td>2.574</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.5</td>
<td>0.987</td>
<td>1.843</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.0</td>
<td>0.762</td>
<td>1.480</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.5</td>
<td>0.620</td>
<td>1.214</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.0</td>
<td>0.541</td>
<td>1.026</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.5</td>
<td>0.464</td>
<td>0.924</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0</td>
<td>0.403</td>
<td>0.806</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.5</td>
<td>0.358</td>
<td>0.717</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.0</td>
<td>0.323</td>
<td>0.645</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.0</td>
<td>0.161</td>
<td>0.323</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(All units in Rydberg)

(a) $n = 10^{26}$ cm$^{-3}$, $T_F = 9.1 \times 10^6$ K

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
TABLE 10
(Units in Rydberg)
(b) \( n = 10^{24} \text{ cm}^{-3} \) \( (T_F = 4.2 \times 10^5 \text{ K}) \)

<table>
<thead>
<tr>
<th>( t )</th>
<th>(-\Omega_x / N)</th>
<th>(-V_x)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.750</td>
<td>1.033</td>
</tr>
<tr>
<td>0.2</td>
<td>0.678</td>
<td>1.008</td>
</tr>
<tr>
<td>0.3</td>
<td>0.606</td>
<td>0.964</td>
</tr>
<tr>
<td>0.4</td>
<td>0.537</td>
<td>0.889</td>
</tr>
<tr>
<td>0.6</td>
<td>0.428</td>
<td>0.751</td>
</tr>
<tr>
<td>1.0</td>
<td>0.299</td>
<td>0.555</td>
</tr>
<tr>
<td>1.5</td>
<td>0.213</td>
<td>0.397</td>
</tr>
<tr>
<td>2.0</td>
<td>0.164</td>
<td>0.319</td>
</tr>
<tr>
<td>2.5</td>
<td>0.134</td>
<td>0.262</td>
</tr>
<tr>
<td>3.0</td>
<td>0.117</td>
<td>0.221</td>
</tr>
<tr>
<td>3.5</td>
<td>0.100</td>
<td>0.199</td>
</tr>
<tr>
<td>4.0</td>
<td>0.087</td>
<td>0.174</td>
</tr>
<tr>
<td>4.5</td>
<td>0.077</td>
<td>0.154</td>
</tr>
<tr>
<td>5.0</td>
<td>0.070</td>
<td>0.139</td>
</tr>
<tr>
<td>10.0</td>
<td>0.035</td>
<td>0.070</td>
</tr>
<tr>
<td>t</td>
<td>-Ω_x/N</td>
<td>-V_x</td>
</tr>
<tr>
<td>----</td>
<td>--------</td>
<td>--------</td>
</tr>
<tr>
<td>0.1</td>
<td>0.162</td>
<td>0.223</td>
</tr>
<tr>
<td>0.2</td>
<td>0.146</td>
<td>0.217</td>
</tr>
<tr>
<td>0.3</td>
<td>0.131</td>
<td>0.208</td>
</tr>
<tr>
<td>0.4</td>
<td>0.116</td>
<td>0.102</td>
</tr>
<tr>
<td>0.6</td>
<td>0.092</td>
<td>0.162</td>
</tr>
<tr>
<td>1.0</td>
<td>0.064</td>
<td>0.120</td>
</tr>
<tr>
<td>1.5</td>
<td>0.046</td>
<td>0.086</td>
</tr>
<tr>
<td>2.0</td>
<td>0.035</td>
<td>0.069</td>
</tr>
<tr>
<td>2.5</td>
<td>0.029</td>
<td>0.056</td>
</tr>
<tr>
<td>3.0</td>
<td>0.025</td>
<td>0.047</td>
</tr>
<tr>
<td>3.5</td>
<td>0.022</td>
<td>0.043</td>
</tr>
<tr>
<td>4.0</td>
<td>0.019</td>
<td>0.037</td>
</tr>
<tr>
<td>4.5</td>
<td>0.017</td>
<td>0.033</td>
</tr>
<tr>
<td>5.0</td>
<td>0.015</td>
<td>0.030</td>
</tr>
<tr>
<td>10.0</td>
<td>0.008</td>
<td>0.015</td>
</tr>
<tr>
<td>t</td>
<td>-Ω_x/N</td>
<td>-V_x</td>
</tr>
<tr>
<td>------</td>
<td>--------</td>
<td>------</td>
</tr>
<tr>
<td>0.1</td>
<td>0.0075</td>
<td>0.0103</td>
</tr>
<tr>
<td>0.2</td>
<td>0.0068</td>
<td>0.0101</td>
</tr>
<tr>
<td>0.3</td>
<td>0.0061</td>
<td>0.0096</td>
</tr>
<tr>
<td>0.4</td>
<td>0.0054</td>
<td>0.0089</td>
</tr>
<tr>
<td>0.6</td>
<td>0.0043</td>
<td>0.0075</td>
</tr>
<tr>
<td>1.0</td>
<td>0.0030</td>
<td>0.0055</td>
</tr>
<tr>
<td>1.5</td>
<td>0.0021</td>
<td>0.0040</td>
</tr>
<tr>
<td>2.0</td>
<td>0.0016</td>
<td>0.0032</td>
</tr>
<tr>
<td>2.5</td>
<td>0.0013</td>
<td>0.0026</td>
</tr>
<tr>
<td>3.0</td>
<td>0.0012</td>
<td>0.0022</td>
</tr>
<tr>
<td>3.5</td>
<td>0.0010</td>
<td>0.0020</td>
</tr>
<tr>
<td>4.0</td>
<td>0.0009</td>
<td>0.0017</td>
</tr>
<tr>
<td>4.5</td>
<td>0.0008</td>
<td>0.0015</td>
</tr>
<tr>
<td>5.0</td>
<td>0.0007</td>
<td>0.0014</td>
</tr>
<tr>
<td>10.0</td>
<td>0.0003</td>
<td>0.0007</td>
</tr>
</tbody>
</table>

TABLE 10
(Units in Rydberg)

(d) \( n = 10^{18} \text{ cm}^{-3} \) (\( T_F = 42.3 \text{ K} \))
<table>
<thead>
<tr>
<th>$t$</th>
<th>$-\Omega_{o}/N_{0}p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>0.4041</td>
</tr>
<tr>
<td>0.1</td>
<td>0.4161</td>
</tr>
<tr>
<td>0.2</td>
<td>0.4610</td>
</tr>
<tr>
<td>0.4</td>
<td>0.5997</td>
</tr>
<tr>
<td>0.6</td>
<td>0.7668</td>
</tr>
<tr>
<td>1.0</td>
<td>1.1312</td>
</tr>
<tr>
<td>1.5</td>
<td>1.6078</td>
</tr>
<tr>
<td>2.0</td>
<td>2.0936</td>
</tr>
<tr>
<td>2.5</td>
<td>2.5839</td>
</tr>
<tr>
<td>3.0</td>
<td>2.0766</td>
</tr>
<tr>
<td>3.5</td>
<td>3.5710</td>
</tr>
<tr>
<td>4.0</td>
<td>4.0664</td>
</tr>
<tr>
<td>4.5</td>
<td>4.5626</td>
</tr>
<tr>
<td>5.0</td>
<td>5.0594</td>
</tr>
</tbody>
</table>
TABLE 12

<table>
<thead>
<tr>
<th>$T$</th>
<th>$-\alpha \psi_{TC}/N$</th>
<th>$-\alpha (e)$</th>
<th>$-\alpha_{XC}/N$</th>
<th>$-\phi_{XC}/N$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.721</td>
<td>0.350</td>
<td>3.829</td>
<td>24.029</td>
</tr>
<tr>
<td>0.6</td>
<td>0.251</td>
<td>0.410</td>
<td>5.975</td>
<td>22.070</td>
</tr>
<tr>
<td>1.0</td>
<td>0.919</td>
<td>0.814</td>
<td>3.751</td>
<td>23.091</td>
</tr>
<tr>
<td>1.5</td>
<td>1.338</td>
<td>1.114</td>
<td>3.903</td>
<td>25.093</td>
</tr>
<tr>
<td>2.0</td>
<td>1.231</td>
<td>2.771</td>
<td>2.200</td>
<td>27.095</td>
</tr>
<tr>
<td>2.5</td>
<td>1.246</td>
<td>2.460</td>
<td>0.990</td>
<td>29.097</td>
</tr>
<tr>
<td>3.0</td>
<td>1.194</td>
<td>2.220</td>
<td>0.853</td>
<td>31.100</td>
</tr>
<tr>
<td>3.5</td>
<td>1.144</td>
<td>2.068</td>
<td>0.807</td>
<td>33.103</td>
</tr>
<tr>
<td>4.0</td>
<td>1.097</td>
<td>1.903</td>
<td>0.767</td>
<td>35.106</td>
</tr>
<tr>
<td>4.5</td>
<td>1.054</td>
<td>1.771</td>
<td>0.732</td>
<td>37.109</td>
</tr>
<tr>
<td>5.0</td>
<td>1.014</td>
<td>1.659</td>
<td>0.701</td>
<td>39.113</td>
</tr>
<tr>
<td>10.0</td>
<td>0.792</td>
<td>1.115</td>
<td>0.530</td>
<td>49.123</td>
</tr>
</tbody>
</table>

$\alpha = 10^{26} \text{ cm}^{-3}$, $T_P = 9 \times 10^6 \text{ K}$

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
TABLE 12

(b) \( n_e = 10^{24} \text{ cm}^{-3} \), \( T_F = 4.2 \times 10^5 \text{ K} \)

<table>
<thead>
<tr>
<th>( t )</th>
<th>(-\nu_c^{(r)})</th>
<th>(-\nu_{xc})</th>
<th>(-\Omega_c^{(r)}/N)</th>
<th>(-\Omega_{xc}/N)</th>
<th>(-\Omega_{o}/N)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.169</td>
<td>1.202</td>
<td>0.177</td>
<td>0.927</td>
<td>1.115</td>
</tr>
<tr>
<td>0.3</td>
<td>0.236</td>
<td>1.200</td>
<td>0.288</td>
<td>0.894</td>
<td>1.407</td>
</tr>
<tr>
<td>0.6</td>
<td>0.382</td>
<td>1.133</td>
<td>0.390</td>
<td>0.818</td>
<td>2.055</td>
</tr>
<tr>
<td>1.0</td>
<td>0.488</td>
<td>1.043</td>
<td>0.429</td>
<td>0.728</td>
<td>3.032</td>
</tr>
<tr>
<td>1.5</td>
<td>0.531</td>
<td>0.928</td>
<td>0.426</td>
<td>0.639</td>
<td>4.309</td>
</tr>
<tr>
<td>2.0</td>
<td>0.534</td>
<td>0.853</td>
<td>0.408</td>
<td>0.572</td>
<td>5.611</td>
</tr>
<tr>
<td>2.5</td>
<td>0.583</td>
<td>0.785</td>
<td>0.388</td>
<td>0.522</td>
<td>6.925</td>
</tr>
<tr>
<td>3.0</td>
<td>0.507</td>
<td>0.728</td>
<td>0.369</td>
<td>0.486</td>
<td>8.246</td>
</tr>
<tr>
<td>3.5</td>
<td>0.490</td>
<td>0.689</td>
<td>0.352</td>
<td>0.452</td>
<td>9.571</td>
</tr>
<tr>
<td>4.0</td>
<td>0.473</td>
<td>0.647</td>
<td>0.337</td>
<td>0.424</td>
<td>10.898</td>
</tr>
<tr>
<td>4.5</td>
<td>0.461</td>
<td>0.615</td>
<td>0.323</td>
<td>0.400</td>
<td>12.228</td>
</tr>
<tr>
<td>5.0</td>
<td>0.443</td>
<td>0.582</td>
<td>0.311</td>
<td>0.381</td>
<td>13.559</td>
</tr>
<tr>
<td>10.0</td>
<td>0.365</td>
<td>0.435</td>
<td>0.240</td>
<td>0.275</td>
<td></td>
</tr>
<tr>
<td>$t$</td>
<td>$-V_C^{(r)}$</td>
<td>$-V_{XC}$</td>
<td>$-\Omega_C^{(r)}/N$</td>
<td>$-\Omega_{XC}/N$</td>
<td>$-\Omega_{\Phi}/N$</td>
</tr>
<tr>
<td>------</td>
<td>--------------</td>
<td>-----------</td>
<td>-------------------</td>
<td>-----------------</td>
<td>-----------------</td>
</tr>
<tr>
<td>0.1</td>
<td>0.093</td>
<td>0.316</td>
<td>0.086</td>
<td>0.248</td>
<td>0.0518</td>
</tr>
<tr>
<td>0.3</td>
<td>0.105</td>
<td>0.313</td>
<td>0.111</td>
<td>0.242</td>
<td>0.0653</td>
</tr>
<tr>
<td>0.6</td>
<td>0.141</td>
<td>0.303</td>
<td>0.141</td>
<td>0.233</td>
<td>0.0954</td>
</tr>
<tr>
<td>1.0</td>
<td>0.175</td>
<td>0.295</td>
<td>0.158</td>
<td>0.222</td>
<td>0.1407</td>
</tr>
<tr>
<td>1.5</td>
<td>0.194</td>
<td>0.280</td>
<td>0.162</td>
<td>0.208</td>
<td>0.2000</td>
</tr>
<tr>
<td>2.0</td>
<td>0.1996</td>
<td>0.269</td>
<td>0.159</td>
<td>0.194</td>
<td>0.2604</td>
</tr>
<tr>
<td>2.5</td>
<td>0.2001</td>
<td>0.256</td>
<td>0.155</td>
<td>0.184</td>
<td>0.3214</td>
</tr>
<tr>
<td>3.0</td>
<td>0.198</td>
<td>0.245</td>
<td>0.150</td>
<td>0.175</td>
<td>0.3827</td>
</tr>
<tr>
<td>3.5</td>
<td>0.194</td>
<td>0.237</td>
<td>0.144</td>
<td>0.166</td>
<td>0.4442</td>
</tr>
<tr>
<td>4.0</td>
<td>0.190</td>
<td>0.227</td>
<td>0.140</td>
<td>0.159</td>
<td>0.5059</td>
</tr>
<tr>
<td>4.5</td>
<td>0.186</td>
<td>0.219</td>
<td>0.135</td>
<td>0.152</td>
<td>0.5676</td>
</tr>
<tr>
<td>5.0</td>
<td>0.181</td>
<td>0.211</td>
<td>0.131</td>
<td>0.146</td>
<td>0.6294</td>
</tr>
<tr>
<td>10.0</td>
<td>0.161</td>
<td>0.176</td>
<td>0.108</td>
<td>0.116</td>
<td></td>
</tr>
</tbody>
</table>

$\Omega_C = 10^{22}$ cm$^{-3}$, $T_F = 2 \times 10^4$ K
\[
\begin{array}{cccc}
\text{TABLE 12} & \text{ } & \text{(d) } n_e = 10^{18} \text{ cm}^{-3}, & T_F = 42.3^\circ \text{ K} \\

\hline
\hline
\text{t} & -V_c^{(r)} & -V_{xc} & -\Omega_c^{(r)}/N & -\Omega_{xc}/N \\
\hline
0.1 & 0.0176 & 0.0279 & 0.0148 & 0.0223 \\
0.3 & 0.0177 & 0.2073 & 0.0152 & 0.0213 \\
0.6 & 0.0185 & 0.0260 & 0.0161 & 0.0204 \\
1.0 & 0.0195 & 0.0250 & 0.0169 & 0.0199 \\
1.5 & 0.0204 & 0.0244 & 0.0174 & 0.0195 \\
2.0 & 0.0210 & 0.0245 & 0.0178 & 0.0194 \\
2.5 & 0.0215 & 0.0241 & 0.0179 & 0.0192 \\
3.0 & 0.0218 & 0.0241 & 0.0180 & 0.0190 \\
3.5 & 0.0221 & 0.0241 & 0.0180 & 0.0189 \\
4.0 & 0.0223 & 0.0240 & 0.0179 & 0.0187 \\
4.5 & 0.0224 & 0.0239 & 0.0179 & 0.0185 \\
5.0 & 0.0223 & 0.0237 & 0.0178 & 0.0185 \\
10.0 & 0.0223 & 0.0230 & 0.0176 & 0.0179 \\
\hline
\end{array}
\]
TABLE 13
NEON SPECTRUM IN A DENSE, HOT PLASMA

N = 10^{24} \text{ electrons/cm}^3, \ T = 100 \text{ eV} = 1.2 \times 10^6 \text{ K}

(atomic units)

<table>
<thead>
<tr>
<th>$\epsilon_i$</th>
<th>$V_{\text{eff}}^I(r)$ (Liberman)</th>
<th>Occupation Probability</th>
<th>$V_{\text{eff}}^II(r)$</th>
<th>Occupation Probability</th>
</tr>
</thead>
<tbody>
<tr>
<td>1s</td>
<td>-30.456</td>
<td>0.9985</td>
<td>-32.653</td>
<td>0.9991</td>
</tr>
<tr>
<td>2s</td>
<td>-2.072</td>
<td>0.236</td>
<td>-2.481</td>
<td>0.256</td>
</tr>
<tr>
<td>2p</td>
<td>-1.360</td>
<td>0.203</td>
<td>-1.948</td>
<td>0.231</td>
</tr>
</tbody>
</table>

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
### TABLE 14

Displaced electron density at the proton

\[ \Delta n = n(0) - n_0 \]

<table>
<thead>
<tr>
<th>Density ( n_0 )</th>
<th>( t = T/T_F )</th>
<th>Self-Consistent L.D.A.</th>
<th>Linear Screening</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Perrot</td>
<td></td>
</tr>
<tr>
<td>( r_s = 1 )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>0.966</td>
<td>0.402</td>
</tr>
<tr>
<td></td>
<td>0.5</td>
<td>0.841</td>
<td>0.365</td>
</tr>
<tr>
<td></td>
<td>1.0</td>
<td>0.682</td>
<td>0.320</td>
</tr>
<tr>
<td></td>
<td>2.0</td>
<td>0.486</td>
<td>0.259</td>
</tr>
<tr>
<td>( r_s = 2 )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>0.478</td>
<td>0.093</td>
</tr>
<tr>
<td></td>
<td>0.5</td>
<td>0.428</td>
<td>0.086</td>
</tr>
<tr>
<td></td>
<td>1.0</td>
<td>0.349</td>
<td>0.077</td>
</tr>
<tr>
<td></td>
<td>2.0</td>
<td>0.235</td>
<td>0.064</td>
</tr>
<tr>
<td>( r_s = 4 )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>0.346</td>
<td>0.022</td>
</tr>
<tr>
<td></td>
<td>0.5</td>
<td>0.338</td>
<td>0.021</td>
</tr>
<tr>
<td></td>
<td>1.0</td>
<td>0.306</td>
<td>0.019</td>
</tr>
<tr>
<td></td>
<td>2.0</td>
<td>0.222</td>
<td>0.016</td>
</tr>
</tbody>
</table>
Fig. 1
\( \int e^{i \mathbf{k} \cdot \mathbf{q}} \mathbf{\hat{r}} \cdot \mathbf{\hat{r}}^2 d^3 r \)

\[ n_0 = 0.68 \times 10^{22} \text{ cm}^{-3} \]
\[ T = 10,000 \text{ K} \]

\[ Q = q/k_T \]

\[ V(Q) \]

**Fig. 2**

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
Fig. 3a
Fig. 3b
Fig. 3c

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
Fig. 4
Fig. 5

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
Fig. 6

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
Fig. 8
Fig. 9
Fig. 10
Fig. 12
$n(r)$
electron cm$^{-3}$

$V_{\text{eff}}(r)$

$t = 0.006$

$t = 2.74$

$n_0 = 10^{24}$ cm$^{-3}$

$V_{\text{xc}}(n_0 T) = -0.37709$ a.u

Fig. 13

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
TABLE CAPTIONS

Table 1(a): Variation of fermi temperature as a function of electron density.

Table 1(b): Typical densities and temperatures of physical systems of interest.

Table 2: Computed values of screening parameters $\xi^2(Q=0,n,t) / \xi_{TF}^2$ and degeneracy parameter $\alpha = \mu / k_B T$ as a function of $t = T / T_F$.

Table 3: Ground state energies for a singly charged impurity (Z=1) in a hot, dense plasma: analysis of Q and T-contributions.

Table 4: 1s, 2s, and 2p energy levels for neon impurity (Z=10) in a plasma at $T = 100$ eV for three different electron densities. The number in parenthesis shows the percentage differences from the corresponding Debye results (units in Rydbergs).

Table 5: The same neon spectrum as in Table 4 at a temperature $T = 750$ eV.

Table 5(a): Comparison of neon Lyman $\alpha(2p\rightarrow 1s)$ line shifts for three plasma densities obtained from the different models discussed in the text. The

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
The linear Debye-Hückel model is the approximation

\[ v_D^L(r) = -\frac{2e^2}{r} \left( 1 - r \xi_D + \frac{1}{2} r^2 \xi_D^2 \right) . \]

The numbers in columns 3 and 6 are from Fig. 3 of Skupsky (1980) (units in Rydbergs).

**Table 5(b):** Comparison of 2s-2p level separation according to various models. The numbers in 3rd and 6th columns are from Fig. 9 of Skupsky (1980).

**Table 6:** Computed neon spectrum using \( V_{IS} \) (Eq. (52) and (54)) (units in Rydbergs). (done by Dr. R. J. W. Henry).

**Table 7:** Energy level spectrum of a singly charged impurity in an electron gas at room temperature (Rydberg units).

**Table 8:** Shallow impurity states at room temperature for singly charged donor impurity in Silicon as a function of carrier density. (Isotropic mass and single-valley degeneracy approximation employed) (units in effective Rydberg = \( e^2/(2a_0\kappa^2) \) with \( \kappa = 11.8 \) for Silicon).
Table 9: Values of the exchange energy and the exchange potential scaled by their respective zero temperature value as a function of t.

Table 10: Values of exchange energy per particle and the exchange potential as a function of t for electron densities (a) $10^{26}$ cm$^{-3}$, (b) $10^{24}$ cm$^{-3}$, (c) $10^{22}$ cm$^{-3}$, and (d) $10^{18}$ cm$^{-3}$.

Table 11: Values of the exchange-correlation potential $V_{xc}$ and the thermodynamic potential $\Omega_{xc}$ as a function of t for several electron densities. Correlation contributions are also listed (all units in Rydbergs).

Table 12: Computed values of the non-interacting part of the thermodynamic potential $\Omega_0$ for a fermi gas as a function of t.

Table 13: Comparison of Kohn-Sham eigenvalues $\epsilon_i$ obtained from self-consistent Hartree scheme of Dr. Liberman for neon in a hot, dense plasma with results obtained using $V_{\text{eff}}^{II}$ (Eq. (97)).

Table 14: Displaced electron density at the site of a proton embedded in an electron plasma for

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
three densities as a function of \( t \). The results of a self-consistent L.D.A. calculation are compared to corresponding linear screening results. All numbers have been taken from Perrot (to appear in Phys. Rev. A (1982)).
FIGURE CAPTIONS

Fig. 1  (a) $\xi_0^2(Q=0,n,t)/\xi_{T_p}^2$ and (b) $\mu/B_p$ versus $t$.

Fig. 2  (a) The effective potential and (b) the associated ground-state form factors as a function of $Q$.

Fig. 3  (a) Behaviour of (A) the effective screened potential $V_{eff}$, (B) the Debye potential $V_D$ and, (C) $V_\xi$ as a function of $r$ in units of Bohr radius at plasma temperature $T = 100$ eV and electron density $n = 4.54 \times 10^{24}$ cm$^{-3}$.

(b) Plot of (A) $V_\xi$ and (B) $V_{eff}$ as a function of $r$ for electron density $n = 4.54 \times 10^{24}$ cm$^{-3}$ and $T = 750$ eV ($t = 7.5$). At this $t$-value, $V_\xi$ merges with $V_D$. $V_{eff}(r)$ has been multiplied by 2 to show the difference which is entirely due to full momentum dependence of $V_{eff}$. (c) The effective screened potential $V_{eff}$ as a function of $r$ for three different plasma densities ($n$) at $T = 100$ eV. (A), $n = 4.54 \times 10^{24}$ cm$^{-3}$ ($t = 1$); (B), $n = 2.47 \times 10^{24}$ cm$^{-3}$ ($t = 1.5$) and (c), $n = 1 \times 10^{24}$ cm$^{-3}$ ($t = 2.74$). The Friedel oscillations are nearly smoothed out for $t = 2.74$.  

131

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
Fig. 4  Neon (Z=10) spectrum at two different plasma temperatures as a function of density. Energy levels supported by (i) $V_{\text{eff}}$ are shown by full lines; (ii) $V_\xi$ by chain lines; (iii) $V_D$ by broken lines. 1a and 1b are 2s and 2p levels in $V_{\text{eff}}$; 2a, 2b, and 3a, 3b are the corresponding energies in $V_\xi$ and $V_D$, respectively.

Fig. 5  Neon Lyman-\(\alpha\) line shifts obtained using $V_{\text{eff}}$ (indicated by \(\Theta\) for three plasma densities at $T=750$ eV compared with corresponding self-consistent results taken from Skupsky's (1980) Fig. 3 \(\Theta\) indicates the corresponding values obtained using Debye potential.

Fig. 6  Plot of 'universal' curves: (a) $\Omega_X[n,T]/\Omega_X[n,0]$. (b) $V_x[n,T]/V_x[n,0]$ as a function of $t = T/T_F$.

Fig. 7  The correlation energy $\Omega^{(r)}_C[n,T]$ (solid curves) and the corresponding exchange energy, $\Omega_X[n,T]$ (broken curves) as a function of $t = T/T_F$ for three different densities (cm\(^{-3}\)). The arrows indicate the values $t_0$ where $V^{(r)}_C$ overtakes $V_X$ (units in Rydbergs).
The exchange-correlation energy $\Omega_{xc}[n,T]$ (solid curves) along with the corresponding exchange contribution $\Omega_x[n,T]$ (broken curves) as a function of $t = T/T_F$ for two densities. Correlation effects are seen to be more important for intermediate and large $t$.

The correlation potential $V^{(r)}_c[n,T]$ (solid curves) and the corresponding exchange potential $V_x[n,T]$ (broken curves) as a function of $t$ for three different densities. The arrows indicate the values $t_o$ where $V^{(r)}_c$ overtakes $V_x$ (units in Rydbergs).

The exchange correlation potential $V_{xc}[n,T]$ (solid curves) along with the corresponding exchange contribution $V_x[n,T]$ (broken curves) as a function of $t$ for two densities. The increased importance of correlation for intermediate and large $t$ is evident.

$V_{xc}[n,T]$ scaled by the respective zero temperature value $V_{xc}[n,0]$ as a function of electron density $n$ (cm$^{-3}$) at three different temperatures.

The cross-over temperature $t_o = T_o/T_F$ as a function of electron density $n$ (cm$^{-3}$). $|V^{(r)}_c|$ >

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
|V_X| above the solid curve while |V_X| > |V_C^{(r)}| below it. The dotted curve distinguishes the corresponding regions for |Ω_C^{(r)}| and |Ω_X|.

Fig. 13 Neon impurity embedded in a hot, dense plasma: surrounding electron density \( n_0 = 10^{24} \text{ cm}^{-3} \), \( T = 100 \text{ eV} \). The schematic plot of (I) the effective potential \( V_{\text{eff}}^{I} \) in the self-consistent Hartree scheme of Dr. Liberman, \( n(r) \) is the corresponding charge density profile. (II) the effective potential \( V_{\text{eff}}^{II} + V_X n(r), T = 100 \text{ eV} \) constructed using the self-consistent \( n(r) \) of (I).
Consider the integral
\[ I = \int_0^\infty \int_0^\infty dx \, dy \, xy \, e^{-t(x^2+y^2)} \, \ln \left| \frac{x+y}{x-y} \right| \]

Let \( x = \sqrt{t} \, u, \, y = \sqrt{t} \, v \),
then \[ I = t^2 \int_0^\infty \int_0^\infty du \, dv \, uv \, e^{-u^2-v^2} \, \ln \left| \frac{u+v}{u-v} \right| \] (A-1)

Now consider
\[ J = \int_0^\infty dv \, v \, e^{-v^2} \, \ln \left| \frac{u+v}{u-v} \right| \]
\[ = - \frac{1}{2} \, e^{-v^2} \, \ln \left| \frac{u+v}{u-v} \right| \bigg|_{v=0}^{v=\infty} \]
\[ + \frac{1}{2} \int_0^\infty dv \, e^{-v^2} \left\{ \frac{1}{u+v} + \frac{1}{u-v} \right\} = u \int_0^\infty \frac{e^{-v^2} \, dv}{u^2-v^2} \] (A-2)

Using (A-2) in (A-1)
\[ I = t^2 \int_0^\infty \int_0^\infty du \, dv \, e^{-u^2-v^2} \, \frac{u^2}{u^2-v^2} \]
\[ = t^2 \int_0^\infty \int_0^\infty du \, dv \, e^{-u^2-v^2} \, \frac{v^2}{u^2-v^2} \] (interchanging \( u \) with \( v \))
\[ = \frac{1}{2} \, t^2 \int_0^\infty \int_0^\infty du \, dv \, e^{-u^2-v^2} \left( \frac{u^2-v^2}{u^2-v^2} \right) = \frac{\pi}{8} \, t^2 \] (upon taking half the sums of the two equivalent expressions)
Appendix B

The second order exchange contribution to grand potential $\frac{\Omega^{(2)}_X}{V_o}$ is given by

$$\frac{\Omega^{(2)}_X}{V_o}$$

$$= \iiint \frac{d^3k}{(2\pi)^3} \frac{d^3p}{(2\pi)^3} \frac{d^3q}{(2\pi)^3} V(q) V(k+p+q) f(k) f(p) (1-f(k+q))(1-f(p+q))$$

$$\varepsilon_{k+q} + \varepsilon_{p+q} - \varepsilon_k - \varepsilon_p$$

where $\varepsilon_k = \frac{\hbar^2 k^2}{2m}$, etc.; $V(q) = \frac{4\pi e^2}{q^2}$ and $V_o$ is the volume of the electron gas at temperature $T$. ($n = N/V_o$). Scaling all momenta by fermi momentum $k_F = (3\pi^2 n)^{1/3}$: $k = xk_F$, $p = yk_F$, $q = zk_F$, we have

$$\frac{\Omega^{(2)}_X}{N}$$

$$= \frac{3}{16\pi^5} \frac{m e^4}{\hbar^2} \iiint \frac{d^3x}{2^2} \frac{d^3y}{2^2} \frac{d^3z}{2^2}$$

$$f(x) f(y) (1-f(x+z))(1-f(y+z))$$

$$\frac{1}{|x+z|^2 + |y+z|^2 - x^2 - y^2}$$

where $f(x) = \frac{1}{e^{\alpha x^2} + 1}$ etc., with $\alpha = \mu/k_BT$.

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
In the high temperature limit: $t \to \infty$

$$f(x) \sim e^{-x^2/t} \ll 1$$

Therefore,

$$\frac{\Omega^{(2)}}{N} \to \frac{3}{16\pi^5} \frac{me^4}{\mu^2}$$

$$e^{2\alpha} \int \frac{d^3x \, d^3y \, d^3z}{z^2 |x+y-z|^2} \frac{e^{-(x^2+y^2)/t}}{(|x+z|^2 + |y+z|^2 - x^2 - y^2)}$$

depends only on $t$.

Noting that $e^{2\alpha} \to \frac{16}{9\pi t^3}$, we have

$$\frac{\Omega^{(2)}}{N} \to \frac{2}{3\pi^6} \frac{1}{t^3} \left( \frac{e^2}{2a_0} \right)$$

$$\int \frac{d^3x \, d^3y \, d^3z}{z^2 |x+y-z|^2} \frac{e^{-(x^2+y^2)/t}}{(|x+z|^2 + |y+z|^2 - x^2 - y^2)}.$$

Scaling $\tilde{x}$, $\tilde{y}$, $\tilde{z}$ by $t^{1/2}$, we get in the high temperature limit $\Omega^{(2)}_x \to \frac{1}{t^{3/2}}$; decaying more rapidly than $\Omega^{(1)}_x$ (which goes as $\frac{1}{t}$).
VITA

Uday Gupta was born on May 22, 1951 in Calcutta, India. He passed the Higher Secondary Examination from Mitra Institution, Calcutta in 1967 and was ranked among the top ten successful students from the State of West Bengal, India in that year. He received the West Bengal State Government Scholarship while studying at Presidency College, Calcutta. He obtained his Bachelor's degree (Physics Honors) from the University of Calcutta in 1970 and his Master's degree in Physics from Indian Institute of Technology, Kharagpur, India in 1973. In 1974, he was a senior Research Scholar (Govt. of India) in the Department of Magnetism, Indian Association for the Cultivation of Science, Calcutta. He obtained his M.S. (Physics) from Carnegie-Mellon University, Pittsburgh, Pennsylvania in 1976. In 1976, he participated in a NATO Summer Institute on "Strongly Coupled Plasmas" in Orleans-la-source, France. He accepted a graduate teaching assistantship in the Department of Physics and Astronomy at Louisiana State University in Baton Rouge, Louisiana, in 1976 where he is currently a candidate for the degree of Doctor of Philosophy.
EXAMINATION AND THESIS REPORT

Candidate: Uday Gupta

Major Field: Many Body Theory (Physics)

Title of Thesis: "Density Functional Formalism"
   I. Finite Temperature Theory
   II. An Atom in a hot, dense plasma

Approved:

[A. K. Rajagopal]
Major Professor and Chairman

[Spencer Geary]
Dean of the Graduate School

EXAMINING COMMITTEE:

[Chen]

[Alvani Bodenhorn]

[RS Goodrich]

[JC Courtney]

Date of Examination: November 20, 1981

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.