Chapter 1

Preview of Thesis

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1.1 INTRODUCTION

To understand different properties of condensed matter system at a microscopic level, knowledge of their atomic structure and dynamics on the basis of realistic interatomic forces is required. The electronic behavior in binary complexes is inevitably much more complex than in one component systems. The advent of binary mixtures has been one of the most exciting events in the field of materials science and engineering. It is observed that such study during the last decade is contributing immensely in the field of condensed matter and materials science. The characteristic behavior of temperature dependent properties of less simple liquids and their alloys generates manifold interest for experimentalists as well as theoreticians. Many quantitative and qualitative theories have been proposed to predict the properties of binary complexes using knowledge of the effective interactions of pure components. Such interactions can be derived in terms of pseudopotential.

Pseudopotential is a method for solving the Schrödinger equation, which contains the essential features of the behaviour of electrons in simple metals. It is defined as
“The artificial but physically justifiable weak effective potential experienced by an electron in the neighborhood of ions and the cloud of surrounding electrons”.

This method is proved useful in studying many properties of metals, alloys, semiconductor and metallic glass. The pseudopotential theory provides insight into virtually every aspects of the behaviour of electrons in a system of condensed matter. From the literature survey it is found that the concept of pseudopotential is well established in the theory of condensed matter, which helps us in understanding various properties including Physical as well as Chemical properties of liquid, crystalline and amorphous materials [1.1-1.8]. It is also known that if one is having a proper and well-stabilized pseudopotential than it yields much better and easier calculations for the different properties of the materials. Still it is interesting to note that inspite of impressive success of pseudopotential theory in solving specific problems; attempts of comprehensive studies are surprisingly rare, even with a local pseudopotential.

Looking to the simplicity of pseudopotential theory- conceptually and computationally, the aim of the proposed Ph. D. thesis entitled “STUDY OF LESS SIMPLE LIQUID ELEMENTS AND THEIR ALLOYS USING PSEUDOPOTENTIALS” is to carryout theoretical
investigations of temperature dependent properties of less simple liquids and their alloys.

1.2 MOTIVATIONS

On the basis of pseudopotential theory, very large number of successful applications are reported so far for the simple as well less simple metals. But the comprehensive study for less simple metals and their binary complexes are not reported in detail. Hence it motivates us to undertake the study on structural dependent transport properties, thermodynamic properties as well of less simple liquids and their binary complexes at various temperatures.

1.3 OBJECTIVES

The main objectives of the present work are as follows:

- Setup a well-characterized model potential which can be used successfully in the investigation of less simple metals and their binary complexes.
- Investigate the structural behaviour of binary mixtures by proposed model potential.
• Study various transport, thermodynamic and dynamical properties of liquid binaries.
• Impact of various local field correction functions on the above mentioned properties.
• Understand the effect of the concentration x as well as temperature on the aforesaid properties in the metallic complexes.

1.4 SCOPE

The well-characterized pseudopotential would be utilized to study various properties of less simple elements and their binary systems, in particular.

This study includes the computation of structural factor and pair correlation function of the liquid state less simple elements and their binaries.

The transport properties viz electrical resistivity, thermoelectric power, thermal conductivity etc. are investigated for the liquid state of less simple elements and their binary mixtures.
Also the investigation of thermodynamic and dynamical properties of such liquid elements and their binaries is carried out.

In addition to these, investigation on the other metallic complexes will be included wherever it is found suitable and convenient to incorporate.

1.5 METHODOLOGY

The present work is purely a theoretical and computational type in nature. The author has completed the literature survey up to the present date before starting the initial work. The initial work was more analytical in nature and it is mainly mathematical formulation of a single parametric local pseudopotential.

To fulfill the objectives and looking to the scope of the present work, various form of the model potentials have been formulated and tested on physical ground. Then a model potential is selected and characterized for its further applications in numeric computations. The necessary computer programs / code are developed, indigenously. These programs are then executed for necessary calculations.
The results emerging from the computations are compared with other such theoretical and experimental data, wherever possible.

1.6 CHAPTERIZATION OF THESIS

To have a qualitative and quantitative picture as well as to draw final conclusions out of a research problem, the proper presentation of the research output plays an important role. Hence in the present study, the author has organized the content of the thesis into various chapters, which include introduction, theory/method of computations and results and discussion part, in general. The atomic distribution in the liquid state is rather irregular compared with that of the solid state. This ambiguous situation hinders the construction of a model for the structure of the liquid state, and thus the liquid state theory appears to progress slowly. Chapters of this Ph. D. thesis deal with the various properties of the liquid complexes. The overview of all the chapters is as follows:

The Chapter-1, in general, deals with the basic definition of the development of pseudopotentials and their capabilities as a tool for
calculating and understanding various properties of matter. It also gives an overview of the whole thesis through chapterization.

The concept of the pseudopotential is narrated in the Chapter-2 of the thesis. A single parametric model potential is proposed [1.9, 1.10] in this chapter. The detailed characterization of the model potential alongwith the determination of the parameter of the electron-ion potential, form factor in real as well as in momentum space is presented. The most fascinating and more advanced screening functions due to Ichimaru-Utsumi (IU) [1.11], Farid et al (FR) [1.12] and Sarkar et al (SS) [1.13] are used to judge screening influence with reference to conventional employed dielectric functions. Also the investigation of pair potentials is carried out. Hence, the analytical work regarding the formulation of the model potential gets completed in this chapter.

After characterizing a model potential, it is used to study some structural analysis of metallic complexes consisting of less simple elements and their binaries. In this respect Chapter-3 provides detailed reporting on the investigations of structure factors S(q) as well as pair correlation functions g(r) of less simple elements using Charged Hard Sphere (CHS) [1.9] approach and their binary mixtures using Aschroft-Langreth (AL)
[1.3], Faber-Ziman (FZ) [1.3] methods. Here the FZ structural dependent transport properties viz. electrical resistivity, thermoelectric power, thermal conductivity etc. were studied and compared with the available experimental data.

The internal energy, entropy and Helmholtz free energy of less simple elements and their binary alloys are investigated on the basis of Gibbs-Bogolouvio inequality [1.14-1.16]. The emerging outcomes therefore are presented in Chapter-4 along with the available experimental results.

Liquid is assumed to have a quasi-crystalline structure for the time periods smaller than the relaxation time even at melting temperature and is characterized by a characteristic time or frequency \( \omega_0 \). In Chapter-5, the computation of the density correlation function, the velocity autocorrelation function and the mean square displacement are reported using the knowledge of the particle position and velocities at various time intervals. The diffusive motion of the atoms in the liquid, which is always present, is described in terms of the linear growth of the mean square distance traveled by the vibrating atoms over a given time. The theory developed by Glass and Rice [1.18] has been successfully used to investigate the dynamical variables of the aforesaid systems.
The concluding discussion of this thesis which summarizes the entire aforesaid work of the present study along with the important general conclusions is narrated in Chapters-6. While giving proper shape of the thesis, however, the necessary discussion and comments/remarks are made at the appropriate point in every chapter in the context of various developments to the current trend in the pseudopotential theory. The scope of further investigations of the work is also narrated in this chapter.

At the end of the thesis further applications of proposed single parametric model potential is explored in Appendices to investigate:

A. Structure factor of Ternary liquid alloys.

B. Electrical resistivity of liquid alkali-group IIIa binary alloys.

C. Superconducting State Parameters (SSP) of amorphous materials.

D. Total Energy, Pressure and Bulk Modulus of BCC alkali metals.
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