C H A P T E R 1

INTRODUCTION

1.I AIM OF THE THESIS

The primary objective of the thesis is to report an investigation about relativistic surface states and allied aspects. As is well known, surface states are bound electron states arising out of vacuum potential discontinuity near the surface of a solid. The relativistic treatment of surface states becomes essential for solids which contain heavy atoms ; this is because the electron motion in such solids requires to be treated on relativistic footing. The use of three-dimensional (3D) models for the purpose of studying surface states relativistically, brings in enormous complexities ; these complexities originate in the intricacies related to three-dimensional Dirac equation which obviously is the basis for studying quantum-mechanically a relativistic electron. As a result the study of relativistic surface states has been considerably dependent on the use of one-dimensional (1D) models [References have been cited at appropriate places in later chapters].

The works reported in the thesis are concerned with relativistic (R) surface states of both semi-infinite and finite systems, together with exploration of some associated features of non-relativistic (NR) surface states. Briefly speaking, the aspects we have investigated are the following :

(A) A study of non-relativistic surface states for semi-infinite systems with surfaces which may contain impurity and distortion, by examining critically as to whether

Kronig-Penney (KP) equation and KP wavefunctions are valid near such surfaces.

(B) Relativistic extension of the studies related to various facets of problems under (A).

(C) Relativistic and non-relativistic surface states and probability densities in semi-infinite systems, with distortion and impurity near the surface.

(D) Relativistic surface states and associated probability density for a finite crystal.

In the next section of the INTRODUCTORY CHAPTER, we put a brief description of how we have presented the materials concerned with investigation of the above-mentioned aspects and some other related situations.

1.II PRESENTATION OF THE INVESTIGATIONS OF THE THESIS

The thesis consists of seven chapters (including this one) and, of course, the bibliography. The chapters 2 and 3 pertain to some non-relativistic studies of surface states, while chapters 4-7 are concerned with relativistic surface states.

In chapter 2, we have discussed some non-relativistic features concerning electron motion in one-dimensional systems in general and surface states in one-dimensional systems in particular ; the situations discussed in this chapter will be found to constitute a basis for comparison of our relativistic results reported in some subsequent chapters.

Chapter 3 is a study of some particular features of NR surface states for semi-infinite systems with surfaces which contain a distortion ; the specific issue considered in this chapter is the question as to whether KP equation and KP wave function can be assumed to be valid near such a surface while one wants to study relevant surface states.

Chapter 4 is a review of investigations of relativistic surface states and some aspects concerned with motion of relativistic electrons in one-dimensional systems. The review provides (i) basic framework for (relativistic) investigations of chapters 5-7 and (ii) several informations with which our relativistic results of chapters 5 and 6 can be fruitfully compared.

Chapter 5 is essentially a relativistic extension of the NR treatment of chapter 3 ; among other things the relativistic results of chapter 5 have been discussed in the light of the NR results of chapter 3.

In chapter 6, our aim has been to report some studies about relativistic surface states and associated probability densities for a semi-infinite system which incorporates both a distortion and an impurity near the surface.

In chapter 7, we have carried out a relativistic study of surface states and associated probability densities of a finite crystal. Some portions of chapter 2 provide the

perspectives regarding the formulation of the relativistic problem of chapter 7.

Besides what has been stated in the preceding paragraphs of this section, chapters 2 - 7 also expose the motivations behind the choices of the aspects of our investigations, and include critical discussion of multifarious results yielded by our studies.

1.III PUBLICATIONS

On the basis of works reported in the thesis, some papers have been already published in journals of international repute and some others have been communicated also to well-known journals. We list below these papers :

P1. Kronig-Penney equation and surface states of a distorted surface, Physica 138B (1986) pp. 141-146.

P2. Relativistic Kronig-Penney equation and Relativistic surface states of a distorted surface, Physica 141B (1986) pp 289-302.

P3. A study of Relativistic Surface States in simultaneous presence of impurity and distortion at the surface, " Revue Roumaine De Physique", (1987), communicated.

P4. Relativistic surface states of a finite crystal, Physica 137A (1986), pp 389-406.

We have enclosed in the beginning of the thesis the copies of the papers which have been already published, namely, P1, P2 and P4. These papers have also been referred to in subsequent chapters at appropriate places. The papers P1-P4, correspond respectively to references [43], [70], [72], [73]. We like to mention that P1 is concerned with chapter 3, P2 is concerned with chapter 5, P3 constitutes the works of chapter 6, and P4 is relevant to the work of chapter 7.

1.IV THE CONCLUDING REMARKS

In concluding the INTRODUCTION to the thesis, we like to mention three important points. The first point is that our intention behind the present chapter is to give the readers of our thesis only a little feeling of what the rest of it is going to deal with. It should not be looked upon as the gist of our thesis.

Secondly, we like to talk about our Bibliography. We have tried our best to include all the references relevant to our thesis. However, it is possible that, inadvertently, we may have missed inclusion of some references. Should this have happened, we beg an unconditional apology.

Thirdly we like to mention some difficulties regarding the pile of symbols we have used in this thesis. As every theoretical physicist would agree, the symbols are essential

dress for any write-up on theoretical physics. To find distinct symbols for every entity coming in our thesis has often proved to be a difficult task. We have tried our best in this regard. Yet, due to unavoidable reasons or oversight, a symbol may have been used in more than one place ; conversely, a particular entity may have been expressed, for convenience, in terms of different symbols in different places. Again, for consistency of presentation of the materials of the thesis, the symbols used in it may be sometimes different from the corresponding ones in the papers we have published. We hope that the contexts in which the symbols have been used are clear enough to prevent any confusion from arising out of the situations just mentioned. Closely connected with issue of symbols is also the question of putting up appropriately the mathematical portions of the thesis. Unfortunately, we are not in possession of the excellent machines which can neatly type out all kinds of symbols and notations one would usually adopt for a thesis like that of ours. Consequently, we have taken recourse to filling by hand certain mathematical parts. In such a process, some errors and omissions are very likely to step in. Again it is our hope that such errors and omissions, if present, will not mean any serious impairment of the clarity and consistency of the materials presented in the thesis.