CHAPTER 1

INTRODUCTION

1.I AIM OF THE THESIS

It becomes necessary to take recourse to relativistic treatments in regard to the motion of electrons in such solids as consist of heavy atoms. The relativistic investigation of the surface states (for solids with heavy atoms), were first undertaken in the decade 1960 - 1970 [the references come in the chapters 4-8] and the problem of relativistic surface states constitutes by now quite an important area of solid state physics. The use of three-dimensional models for the purpose of studying relativistically the surface states and allied aspects, is expected to be involved with enormous complexities ; these complexities would essentially arise out of the intricacies involved with the three-dimensional Dirac equation which obviously forms the basis for studying quantum-mechanically a relativistic electron. As a result, the early works on the relativistic surface states appear to show the trend of using one-dimensional models. And this trend of using one-dimensional models for the study of relativistic surface states has remained in vogue during the entire period spreading from the decade 1960-1970, up to now.

The work of the present thesis was taken up about four years ago. Till that time, the relativistic treatments of surfaces were concerned only with the <u>surface states</u> of (one-dimensional) semi-infinite systems ; they did not consider at all the problem of <u>interface states</u> which are characteristic of the junction of two surfaces. As for the relativistic studies of the surface states (of semi-infinite systems) till about 1979, the surfaces were assumed to be (i) clean, (ii) without any distortion, and (iii) associated with a constant potential in the vacuum region.

In view of the situations narrated in the above paragraph, we based our thesis on three central objectives. They are the following :

(A) A comparative study of some relativistic methods developed for the purpose of studying electron motion in one-dimensional systems.

(B) The relativistic studies of surface states of semi-infinite systems under conditions which are more realistic than the features (i) - (iii) mentioned in the previous paragraph.

(C) The relativistic studies of interface states.

For all the three afore-mentioned objectives, we have made use of one-dimensional models, following the practice then in vogue. The investigation in respect of (A) is carried out by taking recourse to a comparison of certain features of two relativistic approaches. One of these (two) approaches is due to (M.L.) Glasser and (S.G.) Davison

[the reference 34], and the other due to (M.) Steslicka and (S.G.) Davison [the reference 44]; these two approaches have been denoted in the chapters 4-8 as the GD and SD methods respectively. The models considered for the investigation relevant to the objective (A) are based on the use of rectangular well type atomic potential. As for the objective (B) , we have carried out two kinds of investigations ; they are (1) the study of the relativistic surface states of free surfaces of a semi-infinite system, with simultaneous presence of a distortion and an impurity at the surface, and (2) a relativistic treatment of field-sustained surface states (FSSS) of a semi-infinite system, with a clean surface having no distortion. In regard to the objective (C) , we have carried out relativistic generalisations of the well-known Aerts model (page 1063 of the reference 22).

Our studies of various situations corresponding to the above - discussed objectives (A) , (B) and (C) , have led to several fruitful results. These results have exposed clearly how the relativistic corrections in respect of surface states and interface states depend on the kind of methods used, as well as many other relevant circumstances. A detailed discussion of our multifarious findings, which are instructively qualitative and exhaustively quantitative, is given at appropriate places in the remaining parts of the thesis.

It is worthwhile to put in the INTRODUCTORY CHAPTER a brief description of how we have presented the materials of the thesis, and this we do in the next section.

1.II PRESENTATION OF THE INVESTIGATIONS OF THE THESIS

The thesis contains eight chapters (including the present one), one appendix and, of course, the Bibliography. The chapter 2 and 3, are concerned with some non-relativistic studies, while the chapters 4-8 deal with relativistic investigations. The purpose behind the chapter 2 is to review some non-relativistic features relevant to motion of electrons in a one-dimensional system in general, and to surface states in particular; the aspects elucidated in this chapter are necessary for examining comparatively our relativistic investigations in the chapters 4-8. The chapter 3 is a study of the non-relativistic surface states of a particular model; the results of this chapter provide a basis of comparison for those of our relativistic studies in the chapter 6.

The chapter 4 is a review of the relativistic features which are necessary for our (relativistic) studies of the surface states and interface states carried out subsequently in the chapters 5-8.

The chapter 5 is concerned with a comparative study of the GD and SD approaches (objective A in § 1.I). The chapter 6 reports our studies of the surface states of a one-dimensional semi-infinite system with simultaneous presence of an impurity and a distortion at the surface, while the chapter 7 deals with a relativistic investigation of the field-sustained surface states (FSSS) ; the contents of both the chapters 6 and 7 , are relevant to the objective (B) in § 1.I . Lastly, the chapter 8 is pertinent to our study of the relativistic interface states.

Besides what we have stated in the preceeding three paragraphs about the involvements of the chapters 2-8, they include the reviews of pertinent literatures, the exposure of the motivations behind the choices of the aspects of our investigation, and a critical discussion of the findings yielded by our studies.

The lone appendix of our thesis is concerned with the proof of a particular feature of the (two-component) spinor solutions to the one-dimensional Dirac equation ; the feature just mentioned arises in the chapter 4 .