In studying the electrical conductivity, absorption of electromagnetic radiation and similar properties of imperfect solids like the disordered systems or crystalline systems with localised defects, the knowledge about their energy spectrum is very essential. The investigation of energy states of imperfect solids is therefore [redacted] increasing importance. The methods used for such investigations range from those following the "one-electron methods for perfect crystals" to the ones involving field-theoretical techniques. The models studied also vary from simple one dimensional to the general three dimensional cases.

1.2 Outline of the problems investigated and the methods used.

In this thesis, we have investigated the energy states of some one dimensional solids with various types of deviations from periodicity. The problems investigated are the following :

(a) Energy states of one dimensional infinite disordered solid : Several models of infinite one dimensional disordered solid of both mono- and diatomic type have been considered within the frame-work of δ -function and rectangular-well potentials. Two methods have been used for investigating the energy states of these models. One of these methods depends on the use of Green's function in the same way as has been discussed by Saxon and Hutner[1] and Phariseau[2a]. The other method has been developed by us on the basis of boundary conditions to be satisfied by the wave functions at different potential sites. Some models have been studied by both the methods and

the results obtained are identical.

(b) Electronic energy states of edge dislocations : Some results of the investigation about the problems in (a) have been used in studying the effect of edge dislocations on the electronic energy states. The dislocation model has been developed on the basis of a work of Peierls[3].

(c) Energy states of finite solid : By using a matrix method, investigation has been made about the energy states of one dimensional finite solid of pure and mixed type. These investigations have been made within the frame-work of rectangular-well potential. Explicit equations have been derived for allowed energies of several perfect and disordered cases. An analysis has also been made about the criterion for forbiddenness, in a mixed crystal, of any energy which is simultaneously forbidden in the crystals formed by the member atoms separately.

1.3 Survey of investigations and results.

The essentials about the band theory of energy spectrum in solids have been reviewed in chapter II and our investigations about the problems under (a), (b) and (c) have been presented respectively in chapter III, IV and V.

For all the problems treated in (a) and (c), the general approach is to introduce the deviation from periodicity as a perturbation in the interatomic distances. The equations for allowed

energies are then derived in the zeroth and first order approximations. The zeroth order equation gives the energy states of the unperturbed lattice while the first order equation gives the energy-states due to perturbation in the interatomic distances.

To see the quantitative utility of the mathematical derivations, it is necessary to make numerical computations about the location and density of states introduced by perturbation in the interatomic distances. Although most of the equations derived by us are in such a form that one can make numerical calculations on them, we have done the same for only one case namely the problem in (6). This calculation shows in a general way the extent to which the band-structures of energy spectrum are retained in solids with localised defects and the conclusions reached from this calculation are in qualitative agreement with the results of experimental observations.

In chapter V where we have presented investigations about the problems under (c), the superiority of rectangular-well potential over the frequently used δ-function and sinusoidal potential has been discussed. It has been shown that the occurrence of a band-structure in the energy spectrum is closely connected with the properties and particularly the trace of a matrix (which has been named as T-matrix in the text). Out of the T-matrix, two matrices named as t' and S have been constructed and it is shown that the general properties of these matrices are related to the invariance of Schrödinger equation under space-reflection and time-reversal. The T-matrix has been used to derive the equations for allowed energies of several perfect and disordered cases. By using this matrix,

we have also analysed the conditions for forbiddenness, in a mixed crystal, of any energy which is simultaneously forbidden in the member crystals taken separately and our analysis has been discussed in the context of the works done by others on this problem[1,4,5].

More details about results of our investigation for various problems under (a), (b) and (c) have been presented in the summary section of the respective chapters.

Our investigations about the energy states have been made for one dimensional models while in reality, one has to deal with three dimensional systems. A general discussion about the limitations and utility of the results from one dimensional models has been given in chapter III (Section 3.2). In chapter III (Section 3.1), we have also presented a review about the investigations of energy-spectrum in disordered systems by use of such methods as that of numerical calculations, matrix formulation, or perturbational techniques or methods similar to these.

The methods used for investigation of energy states in the works reviewed in chapter III (as mentioned above) are first formulated in most cases for one dimensional systems and then generalised to three dimensional cases. Although results obtained by such methods for one dimensional models are exact, the results for three dimensional systems by generalisation of these methods will be of restricted validity. This is because the mathematical properties peculiar to one dimensional models are not present in three dimensional systems. To overcome this limitation, attempts have been made by many workers to formulate a general theory about the energy-

states of real three dimensional disordered systems by using techniques of quantum-field theory. In chapter VI, we have given an outline of the field-theoretic approach to the study of energy states of disordered systems.