ANALYTIC CONDITIONS FOR THE EXISTENCE OF LOCALIZED ELECTRON STATES IN LINEAR CHAINS WITH TWO IMPURITIES

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The negative eigenvalue theorem is used to obtain an analytic result for the integrated density of electron states in several types of low-dimensional lattices with two impurities in the tight binding approximation. From this expression, analytic conditions for the existence of localized electronic states are obtained. The result is directly applicable to the problem of surface states and that of chemisorption on a linear chain.

1. INTRODUCTION

The linear chain in the tight binding approximation surely represents a drastic simplification of a real three-dimensional solid. Nevertheless, many interesting features, e.g. the existence of localized electron states, are well reflected in this model. Moreover, it is often possible to obtain relevant results much more easily than in more sophisticated models. In addition to it, the problem of electron states (or those of magnons etc.) in thin films may be, in some cases, reduced to a one-dimensional problem, too. Therefore, the results concerning the linear chain are surely important in general.

The problem of localized states is in general tightly connected with that of impurities. In the classical GOODWIN's paper [1], the conditions for the existence of the electron surface states were given for a linear chain with two impurities of the same kind at its ends. GOODWIN's results have been recently generalized by PUSZKARSKI [2] for the case of two different impurities at the ends of the chain. Both these authors used the theory of difference equations. The aim of this paper is to investigate several more general types of lattices with various positions of two impurities and to find out corresponding analytic conditions for the existence of localized states.

So as to derive these conditions, we suggest a new method, based on the negative eigenvalue theorem [3, 4]. This theorem is currently used in numerical calculations [3, 4] but, to our knowledge, it has been never used to obtain any analytic result. Making use of this theorem and applying a suitable unitary transformation to the Hamiltonian in the tight-binding approximation, we succeed to derive an analytic expression for the integrated density of states. From this expression, conditions for the existence of localized impurity state below (or above) the host band of a corresponding ideal infinite chain are obtained. These conditions are then discussed in detail; it is shown that the previous results by GOODWIN [1] and PUSZKARSKI [2] are a special case of our treatment. It is concluded that in many cases the criteria for the existence of localized impurity states in low-dimensional lattices are analogous and may be efficiently discussed in the same way.

2. CONDITIONS FOR THE EXISTENCE OF LOCALIZED STATES

The usual single-electron Schrödinger equation in the tight-binding approximation leads to the following secular equation

\[ Hc = ESc , \]

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where $H$, $S$, $E$ and $c$ are the Hamiltonian matrix, the matrix of overlap integrals, an eigenvalue and a corresponding vector of coefficients determining the true wave function, respectively. For the sake of simplicity, let us take here

\[ H_{ij} = E_0 - \alpha_i \quad \text{for} \quad i = j, \]

\[ -\gamma_{ij} \quad \text{for the nearest neighbours,} \quad \gamma_{ij} > 0, \]

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

and

\[ S_{ij} = \delta_{ij}. \]

Our aim is to investigate the localized states in the six different low dimensional lattices with two impurities which are shown in Fig. 1. The lattices 1–4 are linear chains with two impurities distributed in various ways in the chain. The lattices 5, 6 are not strictly one-dimensional. They may represent a simple model of chemisorption of an adatom (which is denoted by $\alpha_2$) on the linear chain. It is assumed that also the

\[ \text{LATTICE} \]

\[ \text{Fig. 1. Lattices with two impurities.} \]