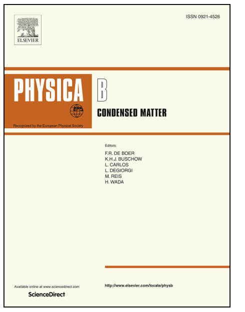
Accepted Manuscript



Band structure of an electron in a kind of periodic potentials with singularities

Kuo Hai, Ning Yu, Jiangping Jia

PII: S0921-4526(18)30240-0

DOI: 10.1016/j.physb.2018.03.039

Reference: PHYSB 310800

To appear in: *Physica B: Physics of Condensed Matter*

Received Date: 16 January 2018

Revised Date: 20 March 2018

Accepted Date: 21 March 2018

Please cite this article as: K. Hai, N. Yu, J. Jia, Band structure of an electron in a kind of periodic potentials with singularities, *Physica B: Physics of Condensed Matter* (2018), doi: 10.1016/j.physb.2018.03.039.

Band structure of an electron in a kind of periodic potentials with singularities

Kuo Hai*, Ning Yu, Jiangping Jia

Department of Physics and Key Laboratory of Low-dimensional Quantum Structures and Quantum Control of Ministry of Education, and Synergetic Innovation Center for Quantum Effects and Applications, Hunan Normal University, Changsha 410081, China

Noninteracting electrons in some crystals may experience periodic potentials with singularities and the governing Schrödinger equation cannot be defined at the singular points. The band structure of a single electron in such a one-dimensional crystal has been calculated by using an equivalent integral form of the Schrödinger equation. Both the perturbed and exact solutions are constructed respectively for the cases of a general singular weak-periodic system and its an exactly solvable version, Kronig-Penney model. Any one of them leads to a special band structure of the energy-dependent parameter, which results in an effective correction to the previous energy-band structure and gives a new explanation for forming the band structure. The used method and obtained results could be a valuable aid in the study of energy bands in solid-state physics, and the new explanation may trigger investigation to different physical mechanism of electron band structures.

Keywords: singular periodic potential, Kronig-Penney model, integral equation, nonphysical divergence, corrected band structure, energy parameter

PACS numbers: 71.20.-b, 03.65.Ge,73.20.At

1. Introduction

One of the fundamental and most important concepts of the physics of solids is the electron band structure [1, 2]. It is the key to understanding the electronic transport and optical properties of solids, such as the difference between metals and insulators or the nature of semiconductors, and the particular phenomena, such as the Hall effect and magnetoresistance. Some different types of band structures [3–8] and the effects of band structure on physical properties [9, 10] have been investigated. Much understanding of the aforementioned points can be obtained through study of a one-dimensional (1D) lattice. The problem of an electron moving in a 1D Kronig-Penney (KP) lattice [11] (a periodic rectangular-well potential or a periodic array of delta functions) can be solved exactly and the solutions were well-discussed in the textbook literature [12–16]. The related problems were further investigated by employing different methods [17–27]. These exact results have demonstrated that the electron states are grouped in bands of allowed and forbidden energies. Particularly, occurrence of a different type of band structure was revealed wherein the Brillouin zone boundaries may not

* Lushan road 36, Changsha 410081, China; Tel. +8615874888778; Email: ron.khai@gmail.com