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

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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 energydependent 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

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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

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