Electron Wave Function in Semiconductor Crystal

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Abstract. The research on semiconductor crystal is a combination of solid-state physics and quantum physics. In this area, Bloch's theorem can be used to describe the periodic structure of crystals, and Schrödinger's equation can be used to describe the energy distribution of free electrons. This paper attempts to combine the two to quantitatively calculate the electron wave function in semiconductor crystals. The main research problem of this paper is to confirm the electron wave function in semiconductor crystals. This paper adopts the method of perturbation theory, using Bloch's theorem and Schrödinger equation to handle with the Kronig-Penney model. Finally, the effective mass of electrons in semiconductor crystals was obtained. This paper uses some advanced mathematical knowledge in this process, such as Taylor expansion and second-order non-degenerate perturbation theory. This mathematical knowledge played a large role in the derivation process. This work demonstrates that the Bloch's theorem serves as a useful approach to handle a series of quantum-mechanical problems in solid-state physics.

Keywords: Semiconductor; Perturbation theory; Bloch's theorem; Kronig-Penney model.

1. Introduction

Semiconductors are the powerful brains behind a variety of modern technology applications, from medical devices and clean energy to transportation and defense. Semiconductor technology is also projected to be a major player in future technology, such as artificial intelligence. If one is to discuss semiconductors, some knowledge of the way electrons move in solids is necessary. First, the way electrons move in a gas can be described by the free-electron gas model, which assumes that electrons travel through a periodic box of vacuum. Extrapolating this model to solids means filling a box with countless atoms and electrons moving around them [1].

A potential well refers to a region in space where a particle experiences a force that tends to confine it. In the context of quantum mechanics, potential wells play a crucial role in understanding the behavior of particles. A one-dimensional potential well is a scenario in which a particle is confined to move along a single dimension, typically the x-axis [2]. The particle's motion is constrained by a potential energy function, which determines the allowed regions for the particle. The one-dimensional finite-depth periodic square well is a model that describes the motion of particles in a periodic potential field with a finite-depth square well. The potential field repeats periodically in space, simulating a periodic lattice structure. Due to the periodic structure, the forbidden energy bands emerge, representing energy ranges where particles cannot exist. Beyond the forbidden bands, there are allowed energy bands where particles can exist. The wave functions describing the particle in the potential field exhibit periodicity, aligning with the periodicity of the potential field [3]. Describes that wave functions in a periodic potential can be written in the form of Bloch waves, where the wave function's form is periodic. Semiconductor is a crystal structure with periodicity. Therefore, the wave function of electrons in semiconductors can be regarded as the wave function of electrons in periodic potential wells.

This paper aims to use the Schrödinger equation and Bloch's theorem to quantitatively calculate the electron wave function in semiconductor crystals. This makes the energy band of the semiconductor crystal structure clearer. In what follows, Sec. 2 presents the models of the one-dimensional potential well and theories of the Bloch theorem. Next, the Kronig-Penney model is shown in Sec. 3.

2. Models and Theories

2.1. One-dimensional Potential Well

In an infinite square well, a particle is confined between two infinite potential barriers. This scenario creates a box-like structure where the particle is free to move within the confines of the potential walls. The infinite square well potential is given by [4]

$$V(x) = \begin{cases} 0, (0 \le x \le a) \\ \infty, (x < 0, x > a) \end{cases} \tag{1}$$

For the illustration of this potential well, see Fig. 1.

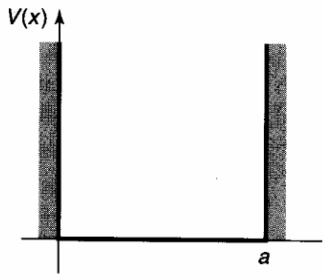

Fig. 1 Illustration of the square potential well.

The one-dimensional finite-depth periodic square well is a model that describes the motion of particles in a periodic potential field with a finite-depth square well. The potential field repeats periodically in space, simulating a lattice structure. Tha author has considered in some detail a particle trapped between infinitely high walls a distance L apart. So the one-dimensional finite-depth periodic square well is given by [5]

$$\begin{cases} V(x) = V_0, (x \le -L/2) \\ V(x) = 0, (-L/2 < x < L/2) \\ V(x) = V_0, (x \ge L/2) \end{cases}. \tag{2}$$

2.2. Bloch Theorem

Felix Bloch, one of the developers of nuclear magnetic resonance, is a Swiss-American physicist who once served as Director General of CERN. In 1952, he and E. M. Purcell won the Nobel Prize in Physics for "*their development of new ways and methods for nuclear magnetic precision measurements.*" Bloch has made great theoretical contributions to the understanding of ferromagnetism and electronic behavior in crystal lattices.

Block theorem. It describes that wave functions in a periodic potential can be written in the form of Bloch waves, where the wave function's form is periodic [6].

Proof. The proof of the Bloch theorem is shown as the following. First, this paper considers a one-dimensional lattice point ring whose geometry is shown in Fig. 2. This only applies to one-dimensional bounded periodic crystals. The period length is a and $V(x) = V(x + as)$.

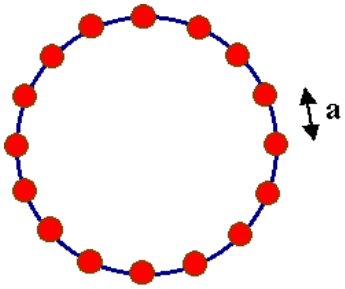

Fig. 2 Illustration of the ring of lattice.

Next, this paper cites the symmetry argument as the decisive idea in this process. There is no difference between the particular coordinate x and the coordinate $(x + a)$, so the difference between the value of $\psi(x)$ and the value at $(x + a)$ will be at most some factor C. Namely,

$$\psi(x + a) = C\psi(x). \tag{3}$$

If it can be proceeded from $(x + a)$ to $(x + 2a)$, it can also be proceeded that $\psi(x + 2a) = \{C^2\}\psi(x)$ and $\psi(x + Na) = \{C^n\}\psi(x) = \psi(x)$. This is because it will be a new round and it will be the same as before. Finally there is $C^N = 1$ and C must be nature number. $C = e^{\frac{i2\pi s}{N}}$ with $s = 0, 1, 2, 3, ..., N - 1$.

There is $\psi(x + a) = \psi(x)e^{\frac{i2\pi s}{N}}$ and if $\psi(x) = u_k(x)e^{\frac{i2\pi xs}{Na}}$, then $u_k(x) = u_k(x + a)$. For u has the lattice periodicity, then it follows that $\psi(x + a) = u_k(x + a)e^{\frac{i2\pi s(x+a)}{Na}}$ and $\psi(x + a) = u_k(x)\, e^{\left(\frac{i2\pi sx}{Na}\right)}e^{\frac{i2\pi s}{N}} = \psi(x)\, e^{\frac{i2\pi s}{N}}$. If it is introduced that $k = 2\pi s\,/Na$ for the one-dimensional case, there is Bloch's theorem. Thus, the Bloch theorem states that [7]

$$\psi_{n,k}(\vec{r}) = e^{i\vec{k}\vec{r}}u_{n,k}(\vec{r}). \tag{4}$$

3. Kronig-Penney Model

Kronig and Penney used a one-dimensional model to describe electrons in periodic electric potentials. The Schrödinger equation is $H\psi = \left(\frac{p^2}{2m} + V\right)\Psi = E\Psi$, and according to the Bloch theorem shown in Eq. (4), it is found that [8]

$$H\psi_{n,k}(\vec{r}) = \left(\frac{p^2}{2m} + V\right)e^{i\vec{k}\vec{r}}u_{n,k}(\vec{r}). \tag{5}$$

For the one dimension case where $p = -i\hbar\theta_x$, it is calculated that

$$H\,\psi_{n,k}(x) = \frac{p^2 e^{ikx}}{2\,m}\;u_{n,k}(x) + Ve^{ikx}u_{n,k}(x) = \frac{\ddot{p}}{2m}\left(\hbar k e^{ikx}u_{n,k} + e^{ikx}\hat{p}.u_{n,k}\right) + Ve^{ikx}u_{n,k}. \tag{6}$$

This Equation can be rewritten as [9]

$$\frac{p^2}{2mu_{n,k}} + \frac{\hbar}{m}(k.p)u_{n,k} + \frac{\hbar^2k^2}{2m}u_{n,k} + Vu_{n,k} = E_{n,k}u_{n,k} \tag{7}$$

and $H_0 = \frac{p^2}{2m} + V$, $H'_k = \frac{\hbar}{m}(k.p) + \frac{\hbar^2k^2}{2m}$. Also, k is a constant vector used to represent periodicity. H_0 is the free electron part of the energy and H'_k is the k-related crystal energy. So the energy at k can be expressed as

$$H_k = -\frac{\hbar^2}{2m}\nabla^2 + V(r) + \frac{\hbar}{m}kp + \frac{\hbar^2k^2}{2m}. \tag{8}$$

If the energy corresponding to k is known, the energy at $k + q$ (q is very small) can be calculated as $H_{k+q} = H_k + \frac{\hbar^2}{m}q\left(\frac{1}{i}\nabla + k\right) + \frac{\hbar^2q^2}{2m}$. The last two items in the above formula can be regarded as perturbation terms δ, which can be obtained from the second-order non-simplified and perturbation theory $E_n^2 \simeq E_n^0 + \delta_{nn} + \sum_{l\neq n}\frac{|\delta_{nl}|^2}{E_n^0 - E_l^0}$. The upper formula can be simplified by Taylor expansion, i.e.,

$$E_n\,(k + q) = E_n(k) + \sum_i \frac{\theta E_n}{\theta k_i}q_i + \frac{1}{2}\sum_{ij}\frac{\theta^2E_n}{\theta k_i\theta k_j}q_iq_j + O(q^3). \tag{9}$$

Finally the equation can be written as [10]

$$\sum_{ij}\frac{1}{2}\frac{\theta^2 E_n}{\theta k_i \theta k_j}q_i q_j = \frac{\hbar^2 q^2}{2m} + \sum_{l\neq n}\frac{\left(\left\langle u_n\left|\frac{\hbar^2 q}{m}\left(\frac{1}{i}\nabla + k\right)\right|u_l\right\rangle\left\langle u_l\left|\frac{\hbar^2 q}{m}\left(\frac{1}{i}\nabla + k\right)\right|u_n\right\rangle\right)}{E_n^0 - E_l^0}. \tag{10}$$

Next, because $p\psi_{nk} = e^{ikr}\hbar\left(k + \frac{1}{i}\nabla\right)u_{nk}(r)$, Eq. (10) can transfer to

$$\frac{1}{2}\sum_{ij}\frac{\theta^2 E_n}{\theta k_i \theta k_j}q_i q_j = \frac{\hbar^2 q^2}{2m} + \sum_{l\neq n}\frac{\frac{\hbar^2}{m^2}(\langle\psi_n|qp|\psi_l\rangle\langle\psi_l|qp|\psi_n\rangle)}{E_N^0 - E_l^0}. \tag{11}$$

Thus, it is inferred that

$$\frac{\theta^2 E_n}{\theta k_i \theta k_j} = \frac{\hbar^2}{m}\delta_{ij} + 2\frac{\hbar^2}{m^2}\sum_{l\neq n}\frac{p_{nl}^i p_{ln}^j}{E_n^0 - E_l^0}p_{nl}^i = \langle\psi_n|p_i|\psi_l\rangle. \tag{12}$$

According to the definition of the effective quality, it is found that [11]

$$(m^*)^{-1} = \frac{1}{\hbar^2}\frac{\theta^2 E}{\theta^2 k}, \qquad \left(\frac{m}{m^*}\right)_{ij} = \delta_{ij} + \frac{2}{m}\sum_{l\neq n}\frac{p_{nl}^i p_{ln}^j}{E_n^0 - E_l^0}. \tag{13}$$

4. Conclusion

This paper first introduces the basic contents of infinitely deep square potential wells and periodic square potential wells as a basis for the semiconductor crystal environment. Next, this paper introduces Bloch's theorem, which is used to quantitatively describe the periodic environment of semiconductor crystals. The above content, coupled with the Schrödinger equation describing the energy distribution of free electrons, satisfies the derivation conditions for the electron wave function in semiconductor crystals. After calculation, the Hamiltonian of electrons in the semiconductor crystal is divided into two parts: free electrons and parts determined by the k value. The paper then performs perturbation analysis on a very small change in the k value, and obtains the effective mass of electrons in semiconductor crystals through second-order non-degenerate perturbation theory and Taylor's theorem. This paper involves many detailed calculations and derivation, making the argument clear at a glance. But there is a lack of practical application of some KP models. In the future, the energy band structure in a certain semiconductor will be determined based on the KP perturbation theory model to create materials more suitable for semiconductors.

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