

Chapter 2

The Model of Kronig and Penney

Abstract Kronig and Penney considered a Meander-like potential energy of the electrons $U(x)$ extended from $-\infty$ until $+\infty$ as a one-dimensional model of a solid. For this model the probability density of electron states has been calculated.

Keyword Kronig-Penney model

As a one-dimensional model of a solid, Kronig and Penney [1] considered a Meander-like potential energy of the electrons $U(x)$ extended from $-\infty$ until $+\infty$. The mathematical description of the potential energy is

$$U(x') = 0 \quad \text{for} \quad 0 < x' < a \quad (2.1)$$

and

$$U(x') = U \quad \text{for} \quad a \leq x' \leq (a + b) = c \quad (2.2)$$

with $x' = x - c$ ($N^A - 1$). The quantity N^A means the number of an atom arranged in the x -direction.

The one-dimensional, time-independent Schrödinger equation for the wave function ψ of the electrons in the considered potential is

$$-\frac{\hbar^2}{2m} \Delta \psi + U(x) \psi = E \psi. \quad (2.3)$$

The symbol $\hbar$ means the reduced Planck's constant, m the mass of an electron, and Δ the Laplace operator, respectively.

The allowed energy levels E of the electrons in the bulk of a body with a periodical potential are placed in the allowed energy bands.

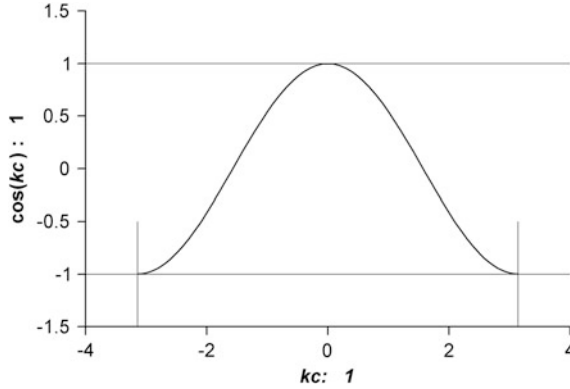


Fig. 2.1 The thick line shows the run of $\cos(kc)$. The horizontal lines at the ordinates $+1$ and -1 are the values of $g(E, U, a, b)$ belonging to the lower and the upper boundaries of the allowed energy band. The short vertical lines mark the values $kc = \pm \pi$

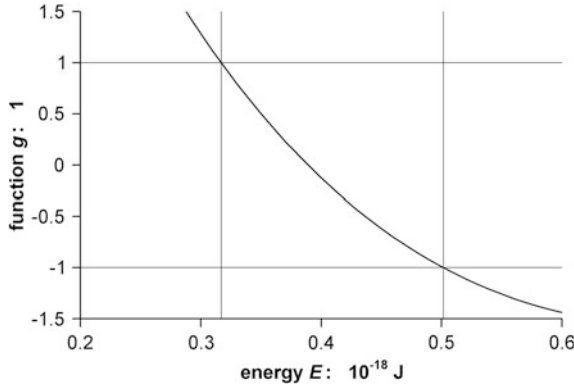


Fig. 2.2 The thick line depicts the run of the function $g(E, U, a, b)$. The horizontal lines at $+1$ and -1 are the values of $g(E, U, a, b)$ at the boundaries of the allowed energy band. The vertical lines mark the lower and the upper boundaries of the allowed energy band

In the energy range $U > E$ follows from the matching conditions for the wave functions the Eq. (2.4)

$$\cos kc = \cos \beta a \times \cosh \gamma b - \frac{\beta^2 - \gamma^2}{2\beta\gamma} \sin \beta a \times \sinh \gamma b = g(E, U, a, b). \quad (2.4)$$

Here k means the wave number, $\beta^2 = \kappa^2 E$, and $\gamma^2 = \kappa^2(U - E)$, respectively. The symbol κ^2 stands for $2m/\hbar^2$.

The fulfillment of Eq. (2.4) is visualized in Figs. 2.1 and 2.2.

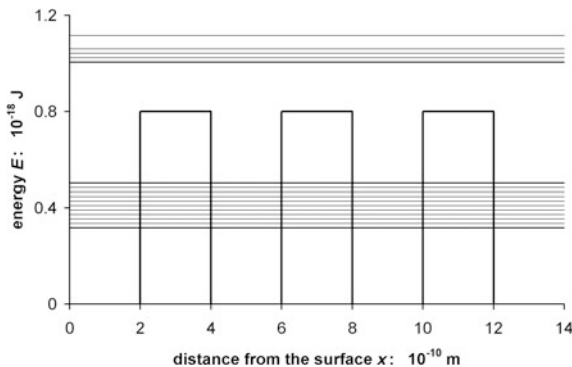


Fig. 2.3 Schematic representation of the run of potential energy in the bulk and of the energy levels in the allowed energy bands (shaded stripes) calculated for a one-dimensional body; (Here, the *thin lines* mark only the range of the allowed energy bands and have no physical meaning.)

In order to find the values of $\pm kc$ corresponding to the energy levels in the allowed energy band, we start in Fig. 2.2 from the abscissa and move vertically upward. From the cross point with the thick curve we shift horizontally to the thick line in Fig. 2.1 and from there vertically down to the abscissa.

In Fig. 2.1, the values of kc corresponding to the energy levels in the allowed energy band are located within the interval

$$-\pi \leq kc \leq \pi. \quad (2.5)$$

The energy eigenvalues have been calculated for $a = 2 \times 10^{-10}$ m, $b = 2 \times 10^{-10}$ m, and $U = 0.8 \times 10^{-18}$ J (5 eV). The energies of the edges of the energy bands are for

- the bottom of the lower energy band: $E^{\text{Bl}} = 0.317 \times 10^{-18}$ J.
- the top of the lower energy band: $E^{\text{Tl}} = 0.502 \times 10^{-18}$ J.
- the bottom of the upper energy band: $E^{\text{Bu}} = 1.005 \times 10^{-18}$ J.
- the top of the upper energy band: $E^{\text{Tu}} = 1.880 \times 10^{-18}$ J.

The three lowest band edges are depicted in Fig. 2.3.

2.1 The Density of the Electron Energy Levels $n(E)$

The motion of the quasi-free electrons in a periodic potential is described by the wave number k , defined by

$$k = \frac{2\pi}{L}n. \quad (2.6)$$

Generally speaking, L is the observation abstraction for the length of an oscillating system. In the infinitely extended body, the quantity L means an arbitrary length the one-dimensional body is subdivided in. With other words, the infinitely extended body is composed by a periodical repetition of subranges with the length L in the x -direction. The value of L limits the number of the wave functions per energy band but it does not limit the extension of the wave functions.

For each wave number vector an oppositely directed wave number vector exists

$$|\vec{k}| = |\vec{k}|. \quad (2.7)$$

Without regard to the spin, it follows for the number of the energy levels in the allowed energy band

$$n = 2 \frac{L}{2\pi} k. \quad (2.8)$$

By differentiation of Eq. (2.8) with respect to the energy E we obtain for the density of states in an allowed energy band

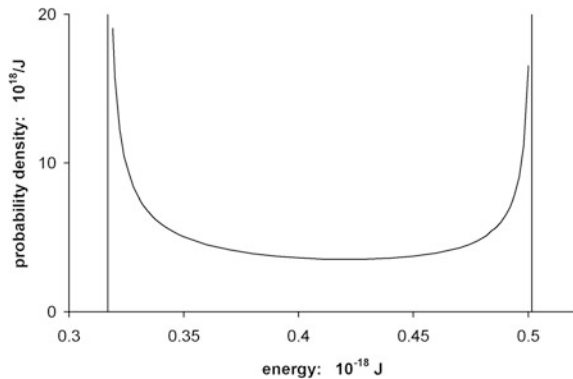
$$n(E) = \frac{dn}{dE} = \frac{L}{\pi} \frac{dk}{dE}. \quad (2.9)$$

In an infinitely extended solid with its infinite number of atoms, infinitely many different values of the wave number k exist. Therefore, the density of the allowed energy levels is infinitely large too. For this situation, it is only meaningful to use the probability density for the existence of an electron state with the energy E

$$p(E) = \lim_{N \rightarrow \infty} \frac{1}{N} \frac{dn}{dE} = \lim_{N \rightarrow \infty} \frac{1}{N} \frac{L}{\pi} \frac{dk}{dE}. \quad (2.10)$$

Figure 2.4 shows the probability density of electron states $(c/L)n(E)$ for the energy E .

Fig. 2.4 The probability density of electron states $(c/L)n(E)$ for a one-dimensional body versus the energy E



2.2 Remarks

The mean value $(a + b)/2 = 2 \times 10^{-10}$ m is comparable with the radius of sodium atoms. That means, the number of atoms along an edge of a cube with a length of $L = 1$ m is 2.5×10^9 atoms.

For the potential barrier U in the bulk a value near the ionization potential of sodium has been chosen.

The applied method for the theoretical calculations is a separable crystal potential in the one-electron Schrödinger equation.

In the Kronig–Penney model there is no statement concerning the position of the Fermi level. Therefore, the model of the solid can be adapted to bodies with different physical properties.

Reference

1. de Kronig RL, Penney WG (1931) Quantum mechanics of electrons in crystal lattices. Proc R Soc 130(Ser A):499–513

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