SURFACE STATES IN ONE-DIMENSIONAL MODEL OF A CRYSTAL WITH AN EXTERNAL FIELD

By J. Peisert

Institute of Mathematics, Technical University of Wrocław*

(Received December 30, 1975; revised version received October 12, 1976)

The approximate formula for the number of surface states has been obtained for the model of a one-dimensional semi-infinite crystal with an arbitrary potential at the boundary and the Kronig-Penney-type potential inside the crystal.

1. Introduction

It is well-known from the theory of surface states [1], that in the crystal model in which the rectangular barrier is taken as a boundary potential, at least one surface state is obtained in each forbidden zone of the crystal electron spectrum. Flores, Louis and Rubio [2] studied the influence of the potential shape in the intermediate region between the undeformed crystal and the vacuum in the case of the linear barrier and afterwards Garcia and Solana [3], for the case of the image potential barrier. The first result of these investigations was the general conclusion that the number of surface states depends on the potential barrier shape. In the case of the linear barrier of intermediate region width l, it has been found that the second surface state appears in the forbidden zone of a semiconductor when $l \gtrsim 3$Å. In the work of Garcia [3], the surface states spectrum dependence on the value of the parameter C in the image potential $V(x) = -\frac{Ce^2}{x}$ was analyzed. With physically reasonable fixed values of the lattice constant a and of the potential barrier depth V_0, it has been shown that an increase in C is accompanied by an increasing number of surface states, first in the energy gap nearest to the vacuum level and next in the second gap. Similarly as in the work of Flores [2], the authors get their results numerically, using the Bessel function as an approximation of the Whittaker function which is a solution of the Schrödinger equation with the Coulomb potential.

* Address: Instytut Matematyki, Politechnika Wrocławska, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland.

Kolař and Bartoš [4] obtained further results in the semi-infinite one-dimensional crystal model with a sinusoidal potential of $2|V|\cos\frac{2\pi}{a}(x-x_0)$ type inside, and image potential $\frac{C}{x-x_1}+V_0$ outside the crystal. For the values (a.u.) $a=\pi$, $|V|=0.02$, $C=0.5$ and various values of V_0 the most interesting result of numerical calculations was obtained for V_0 tending to $\left(\frac{\pi}{a}\right)^2+|V|$, where it has been found that the surface states number tends to infinity.

2. *The model*

The subject of the present work is an analytic investigation of the dependence between the surface potential shape, particularly its asymptotics, and the existence and number of surface states in the one-dimensional model of the semi-infinite crystal.

We consider the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]u(x,E)=Eu(x,E), \qquad 0<x<\infty$$

with the potential $V(x)$ tending to V_0+Fx as $x\to\infty$ (Fig. 1). The potential describes, for example, the field ionization case. It was analyzed by Stęślicka [5] for $V(x)$ exactly

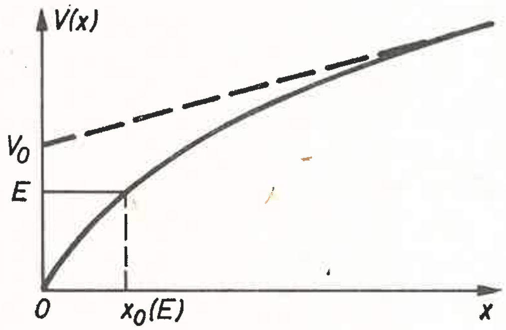

Fig. 1. The potential energy shape with the classical turning point $x_0(E)$

equal to V_0+Fx. If we use the Kronig–Penney potential for the interior of the crystal then the surface states energy value equation has the form

$$ka\operatorname{ctg}ka+\frac{k^2a^2}{P}=-\frac{a^2f^2(E)}{P}-af(E), \tag{1}$$

where P is the power of the Dirac delta describing the potential well, a is the lattice constant and $f(E)$ is the logarithmic derivative of $u(x,E)$ for $x=0$. Solutions of this equation are the surface states, subject to

$$f(E) < -\frac{P}{2a}, \tag{2}$$

which is the "existence condition" obtained identically as the Tamm condition for the rectangular barrier model [1].

3. Calculations

It is known from the theory of ordinary differential equations [6] that the solution $u(x)$ has an oscillatory character for $E-V(x) > 0$. In the case of the Schrödinger equation with the potential as in Fig. 1 the function $E-V(x)$ is negative for $x > x_0(E)$ and positive for $x < x_0(E)$. So, in the last case the solution is oscillating. The zeros of $u(x)$ are placed only in the region $0 \leqslant x < x_0(E)$. The number of zeros is given by the approximate formula [6]

$$N(x_0) \approx \frac{1}{\pi}\int\limits_0^{x_0(E)} dx\left\{\frac{2m}{\hbar^2}[E-V(x)]\right\}^{\frac{1}{2}}, \tag{3}$$

and it is of course a function of energy E.

In can be seen from equation (1) that knowledge of the $f(E)$ function singularities, i.e. of $u(0, E)$ zeros, plays an essential role in this problem. On the other hand, it is easy to find the number of zeros in the region $0 \leqslant E < E_0$ is equal to the number of zeros of $u(x, E)$ in the region $0 \leqslant x < \infty$. It is also possible to show, that $f(E)$ has always the positive derivative and it may be written as the tangent of a continuous monotonic function. As the "density" of $f(E)$ singularities is determined by (3), we represent our function by

$$f(E) \sim \operatorname{tg}\left[\int\limits_0^{x_0(E)} dx\left\{\frac{2m}{\hbar^2}[E-V(x)]\right\}^{\frac{1}{2}} + A\right].$$

We can estimate the constant A requiring that

$$f(E) \approx f_0(E) = -\left[\frac{2m}{\hbar^2}(V_0-E)\right]^{\frac{1}{2}}$$

as E tends to zero from above, when $f_0(E)$ is the exact function $f(E)$ for the rectangular barrier model.

Finally, the function $f(E)$ is equal to

$$f(E) \approx \left[\frac{2mV_0}{\hbar^2}\right]^{\frac{1}{2}} \operatorname{tg}\left\{\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \int\limits_0^{V^{-1}(E)} dx[E-V(x)]^{\frac{1}{2}} - \frac{\pi}{4}\right\}. \tag{4}$$

The graphs of the left and right hand sides of (1) are sketched in Fig. 2, and it was easy to assume that the maximal values of the right side of (1) have the common value $P/4$ independently of a. The method used above is closely connected with the WKB method.

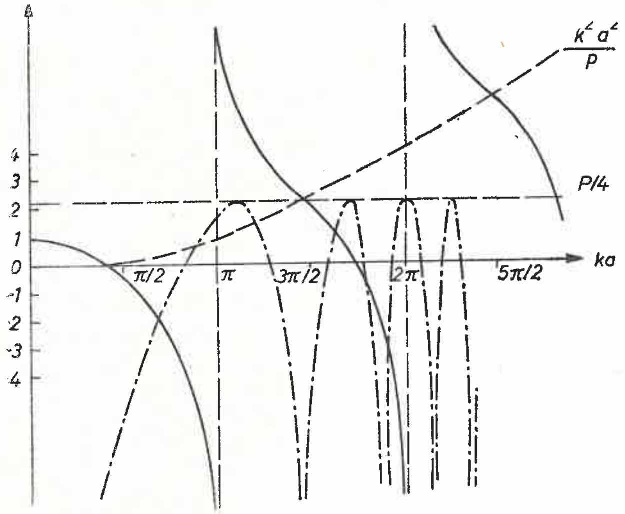

Fig. 2. The trace of equation (1). The solid and the dotted lines correspond to the left and right hand sides respectively. Here $P = 3\pi$

4. *Results*

Now we can represent the expression for the surface states number in the succesive n-th energy gap. We should notice that each singularity of $f(E)$ produces in general two roots of (1) (rarely one root). Yet is it easy to prove that condition (2) is fulfilled only for the right side of (1) having the positive derivative. So, each singularity of $f(E)$ gives in general one surface state if only E is taken from the energy gap.

Let E_n^0 denote the lower limit of the n-th energy gap,

$$E_n^0 = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2$$

and let

$$E_n = \frac{\hbar^2}{2m} k_n^2,$$

where k_n is the n-th positive root of the equation

$$ka \operatorname{ctg} ka + \frac{k^2a^2}{P} = \frac{P}{4}.$$

Then, the number of surface states in the n-th forbidden zone is approximately

$$l_n \approx 1 + N(E_n) - N(E_n^0), \tag{5}$$

where $N(E) \equiv N(x_0(E))$ is given by (3). The number 1 appearing in the above formula is introduced for the case when $f(E)$ is continuous, and then the cotangent singularity gives the root of (1).

Let us examine the influence of asymptotics of the potential on the existence and number of surface states. For $F = 0$, $f(E)$ has a finite number of singularities if $N(V_0)$ has a finite value i.e. when the integral

$$\int_0^{\infty} dx[V_0 - V(x)]^{\frac{1}{2}} \tag{6}$$

is finite. In the opposite case, including the image potential case, the divergence of (6) gives an infinite number of singularities of $f(E)$ with the accumulation point V_0. Now, if the parameters a and P are such that V_0 is found inside the energy gap, we get an infinite number of surface state energy levels.

For $V(x) = V_0 + Fx + V_1(x)$, $V_1(x) \to 0$ as $x \to \infty$, the formula (3)

$$N(E) \approx \frac{1}{\pi}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \int_0^{x_0(E)} dx[E - V_0 - Fx - V_1(x)]^{\frac{1}{2}}$$

exhibits that for $F \neq 0$, $N(E)$ is finite only if $x_0(E)$ exist. So, if $F > 0$, then l_n estimate the number of "real" surface states, and in the opposite case ($F < 0$) — "virtual" surface states considered by Modinos [7], which does not exist in a static case due to tunneling. For small F the problem reduces to the previous one ($F = 0$). For large $F > 0$ we have

$$x_0(E) = \frac{1}{F}[E - V_0 - V_1(x_0)] \approx \frac{1}{F}[E - V_0 - V_1(0)]$$

and

$$N(x_0(E)) \to 0 \quad \text{when } F \to \infty.$$

5. Final remarks

To conclude, we have got in analytical way the general expression for the number of surface states in the one-dimensional semi-infinite crystal model with the Kronig-Penney potential inside the crystal and an arbitrary monotonic one outside. We have generalized the results [2–4] presented at the beginning, for the arbitrary boundary potential. The presented expresions are not valid for small energies E, but the last case is well described by the rectangular barrier model.

In one physically significant case of image-force potential

$$V(x) = V_0 - \frac{e^2}{4(x + x_0)}, \quad x_0 > 0$$

the exact number of zeros of the solution $u(x, E)$ of the Schrödinger equation may be given, but only in the region $-x_0 < x < \infty$ [8]. It is

$$N(E) = \mathrm{int}\left[\frac{me^4}{32\hbar^2(V_0-E)}\right]^{\frac{1}{2}}.$$

However, this formula can be used as a good approximation for the calculation of the number of surface states (5).

We think that the use of a potential other than the Kronig-Penney does not introduce any substantial change in the formulas.

The author would like to thank Professor K. F. Wojciechowski for constant encouragement and advice and dr M. Stęślicka for the essential remarks.

REFERENCES

[1] S. G. Davison, J. D. Levine, *Surface States*, Academic Press, New York and London 1970.
[2] F. Flores, E. Louis, J. Rubio, *J. Phys.* **5**, 3469 (1972).
[3] N. Garcia, J. Solana, *Surf. Sci.* **36**, 262 (1973).
[4] M. Kolař, I. Bartoš, *Czech. J. Phys.* **B23**, 179 (1973).
[5] M. Stęślicka, *Phys. Lett.* **57A**, 255 (1976).
[6] P. Hartman, *Ordinary Differential Equations*, J. Wiley, New York 1964, Sec. XI.
[7] A. Modinos, *Surf. Sci.* **5**, 157 (1975).
[8] H. Bateman, A. Erdélyi, *Higher Transcendental Functions*, Mc Graw-Hill, New York-Toronto--London 1953, vol. 1, Ch. 6, § 6. 16, Fig. 7.