A numeric Study on the Influence of the Values of the Parameter P in Kronig – Peneny Equation on the Width of the Bands

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Abstract

After showing the importance of Bloch Theory about Schrödinger' equation solution with a periodic potential; we demonstrated that the periodic structure of square well in one dimension of the model of Kronig-Penney on the band theory of solid, shows clearly the structure of the allowed and forbidden bands in the in the crystalized solids and we showed how we can introduce the parameter p in the final equation of this model of bands. Then, we conducted a sufficient study on the influence of this parameter on the widths of the allowed and forbidden energy bands in the crystals. We find that, the width of an allowed band decreases with the increase in the value of this parameter, and the width of a forbidden band increases with the increase in the value of this parameter.

Keywords: periodic potential, Bloch function, energy band, allowed (range) band, forbidden (range) band.

Introduction:

In 1928 Bloch has proved the important theorem that the solutions of the Schrödinger equation with a periodic potential are, in three dimensions, of the form [1, 2, 3 , 4] :

$$\varphi_k(\vec{r}) = u_k(\vec{r})\exp(i\vec{k}.\vec{r}) \qquad (1)$$

In one dimension , the solutions are reduced to an expression of the form [1] :

$$\varphi_k(x) = u_k(x)\exp(ikx) \qquad (\acute{1})$$

Where $u_k(\vec{r})$ and ($u_k(x)$) are functions depending on the wave vector $\vec{k}$; (on the wave number k , respectively , which is periodic in x, y, and z ; (which is periodic in x) , with the periodicity of the potential , that is with the period of the lattice of the crystal . The solutions of the form (1) ; and (of the form ($\acute{1}$) , are known as Bloch functions in three dimensions ; (in one dimension). We see that a Bloch function is a plane wave: ($\exp(i\vec{k}.\vec{r})$) which is modulated with the period of the lattice.

Since that date , the Bloch functions were largely used in the study of the solid state , especially in the study of the propagation of waves associated with the motion of electrons and holes in the crystals [1 , 2, 3 , 5 , 6 , 7, 8 , 9 , 13 , 14 , 15 , 16, 17] .

If we consider N lattice points on a ring of length Na , with $N \longrightarrow \infty$; and if we suppose that the period of the potential is a , so that :

$V(x) = V(x + ga)$, where g is an integer,

Then, because of the symmetry of the ring , we look for eigen-functions $\varphi(x)$ such that :

$\varphi(x + a) = c\varphi(x)$,

Where c is a complex constant , then , [3 , 5 ,6 , 7 , 9 ,15] we have :

$\varphi(x + ga) = c^g \varphi(x)$;

and , if the eigen-function is to be single-value, then :

$\varphi(x + Na) = c^N \varphi(x) = \varphi(x)$,

so that c is one of the N roots of the unity [3, 6 , 7 , 9, 15] , then :

$c = \exp(i2\pi g/N)$; $g = 0, 1, 2, 3, \ldots\ldots, N-1$.

So that the Bloch function in one dimension is writing :

$$\varphi(x) = \exp(i2\pi gx/(Na))\, u_g(x) \qquad (2)$$

where $u_g(x)$ has the periodicity a of the linear lattice , and if we write :.

$k = 2\pi g/(Na)$,

then , the Bloch function in one dimension , which a satisfactory solution of Schrödinger wave equation, in one dimension is given by the expression :

$$\varphi_k(x) = \exp(ikx)u_k(x) \qquad (3)$$

At the beginning of this research , we showed the expressions of Schrödinger wave equations used for the one dimensional periodic potential of the model of Kronig - Penney [6 , 7 , 10, 12, 15]. Then , after we had found the expression of the determinant of the system of the four linear homogeneous equations obtained from the equations of Schrödinger for the model, we wrote the condition on this determinant which gives the acceptable solutions of the four linear homogeneous equations . After that we gave the expression of the parameter p [6 , 7, 10, 12, 15] , then we established the handier equation of the model of Kronig- Penney which contain the parameter p and which determines the ranges of allowed and forbidden bands of the energy E [6 ,7, 10 ,12, 15] . At the end of this research we gave a large numeric study on the influence of values of

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the parameter p on the widths of the allowed bands and forbidden bands of energy in the crystalized solids .

Kronig-Penney model:

In this model , largely used in the band theory of solids , we dealt with a periodic square-well potential in one dimension (see figure 1). This model is largely artificial , but it is a model which can be treated explicitly , using only elementary functions, and we could with this model, demonstrate some of the fundamental characteristic features of electron propagation in crystals [5 , 6 , 10 , 12 , 17] .

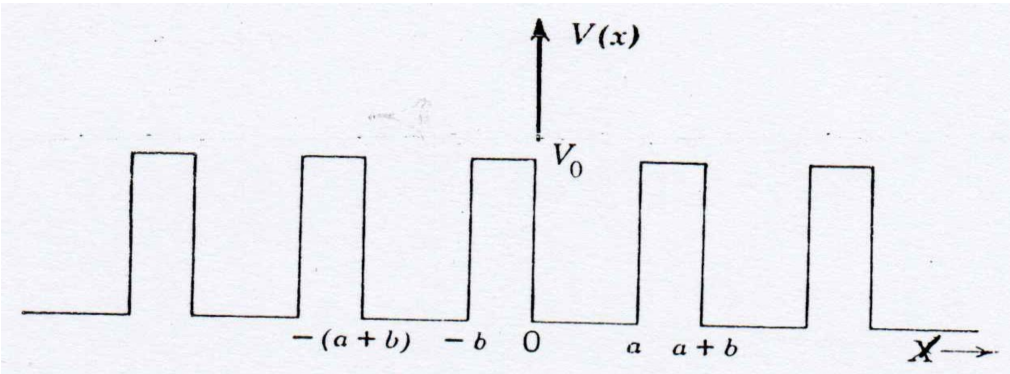

Fig.1 : Kronig and Penney one dimensional periodic potential.

The Schrödinger wave equation of the problem is:

$\frac{d^2\varphi(x)}{dx^2} + \frac{2m}{\hbar^2}(E - V)\varphi(x) = 0$ (4)

The running wave solutions will be of the form of a plane wave modulated with the periodicity of the lattice.

By substituting (3) into (4), we get ,

$\frac{d^2u(x)}{dx^2} + 2ik\frac{d\,u(x)}{d\,x} + \frac{2m}{\hbar^2}(E - E_k - V)u(x) = 0$ (5)

where $E_k = \hbar^2k^2/(2m)$

In the region : $0 \le x \le a$; and in the regions which are equivalent to this region , (for example , the region : $-(a+b) \le x \le -b$; see the figure 1), the general solution of the equation (5) has the form [4 , 6 , 7 , 11] :

$u_{1k}(x) = A\exp[i(\alpha - k)x] + B\exp[-i(\alpha + k)x]$ (6)

Where we pose : $\alpha = [2mE/\hbar^2]^{1/2}$, and (7)

A and B are two constants of integration.

In the region : $a \le x \le a + b$; and in the regions which are equivalent to this region, (for example , the region : $-b \le x \le 0$; see the figure 1), the general solution of the equation (5) has the form [4 , 6 , 7 , 11] :

$u_{2k}(x) = C\exp[(\beta - ik)x] + D\exp[-(\beta + ik)x]$ (8)

Where we pose : $\beta = [2m(V_0 - E)/\hbar^2]^{1/2}$, and (9)

C and D are two constants of integration .

From the continuity of the wave functions at the points : x = 0 and x = a , we have respectively : $u_{1k}(0) = u_{2k}(0)$, and ; $u_{1k}(a) = u_{2k}(a)$; then we get , respectively ,

$A + B - C - D = 0$ (a)

and

$[e^{i(\alpha - K)a}]A + [e^{-i(\alpha + k)a}]B - [e^{(\beta - ik)a}]C - [e^{-(\beta + ik)a}]D = 0$; ($\acute{b}$)

and from the continuity of the derivatives of the wave functions at the points : x = 0 and x = a ; we have , respectively : $(du_{1k}/dx)_{x=0} = (du_{2k}/dx)_{x=0}$, and; $(du_{1k}/dx)_{x=a} = (du_{2k}/dx)_{x=a}$; then we get , respectively,

$[i(\alpha - k)]A - [i(\alpha + k)]B - [(\beta - ik)]C + [(\beta + ik)]D = 0$; (c)

and

$[i(\alpha - k)e^{i(\alpha - k)a}]A - [i(\alpha + k)e^{-i(\alpha + k)a}]B - [(\beta - ik)e^{(\beta - ik)a}]C + [(\beta + ik)e^{-(\beta + ik)a}]D = 0$. ($\acute{d}$)

The periodicity of $u_{1k}(x)$ and $u_{2k}(x)$ and of their derivatives requires that the values of $u_{1k}(x)$ and $u_{2k}(x)$ and of (du_{1k}/dx) and (du_{2k}/dx) at the point x = a must be equal to those at the point x = -b , then we have : $u_{1k}(a) = u_{2k}(a) = u_{2k}(-b)$ and $(du_{1k}/dx)_{x=a} = (du_{2k}/dx)_{x=-b}$; then we rewrite the equations ($\acute{b}$) and ($\acute{d}$) , respectively , as follows :

$[e^{i(\alpha - K)a}]A + [e^{-i(\alpha + k)a}]B - [e^{-(\beta - ik)b}]C - [e^{(\beta + ik)b}]D = 0$; (b)

and

$[i(\alpha - k)e^{i(\alpha - k)a}]A - [i(\alpha + k)e^{-i(\alpha + k)a}]B - [(\beta - ik)e^{-(\beta - ik)b}]C + [(\beta + ik)e^{(\beta + ik)b}]D = 0$. (d)

The constants A , B , C and D must be chosen in such a manner that the four conditions giving by the equations : (a) , (b) , (c) and (d) are satisfied , then the wave functions may be calculated by determining the values of these precedents constants . However, here we are more interested

in determining the values of the energy E for which satisfactory solutions are obtained ,then :
if we put :
$d_{11} = 1$; $d_{12} = 1$; $d_{13} = -1$; $d_{14} = -1$; $d_{21} = i(\alpha - k)$; $d_{22} = -i(\alpha+k)$; $d_{23} = -(\beta-ik)$; (10a)
$d_{24} = (\beta + ik)$; $d_{31} = e^{i(\alpha - k)a}$; $d_{32} = e^{-i(\alpha + k)a}$; $d_{33} = -e^{-(\beta - ik)b}$; $d_{34} = -e^{(\beta + ik)b}$; (10b)
$d_{41} = i(\alpha - k)e^{i(\alpha - k)a}$; $d_{42} = -i(\alpha + k)e^{-i(\alpha+k)a}$; $d_{43} = -(\beta - ik)e^{-(\beta - ik)b}$ and $d_{44} = (\beta+ik)e^{(\beta + ik)b}$ (10c)
then, we will be able to rewrite the precedent system of the four linear homogeneous equations : (a), (b), (c) and (d) as follows:

$$\begin{vmatrix} d_{11} & \dots & d_{14} \\ \cdot & \dots & \cdot \\ \cdot & \dots & \cdot \\ d_{41} & \dots & d_{44} \end{vmatrix} \begin{vmatrix} A \\ B \\ C \\ D \end{vmatrix} = \begin{vmatrix} 0 \\ 0 \\ 0 \\ 0 \end{vmatrix} \qquad (11)$$

Here , we are not interested in the determination of the solutions (6) and (8) of the running waves in the periodic potential in one dimension of the model which are obtained by determining the values of constants : A , B , C and D which determine the solution of the system (11) of the four linear homogeneous equations , but we are more interested here in finding the values of the energy E for which satisfactory solutions can be obtained , from which we can determine the limits of the bands of energy in the solid .
The determinant of the system (11) of the four linear homogeneous equations is written as:

$$\begin{vmatrix} d_{11} & d_{12} & d_{13} & d_{14} \\ d_{21} & d_{22} & d_{23} & d_{24} \\ d_{31} & d_{32} & d_{33} & d_{34} \\ d_{41} & d_{42} & d_{43} & d_{44} \end{vmatrix} = (-1)^{1+1} d_{11} \begin{vmatrix} d_{22} & d_{23} & d_{24} \\ d_{32} & d_{33} & d_{34} \\ d_{42} & d_{43} & d_{44} \end{vmatrix} + (-1)^{1+2} d_{12} \begin{vmatrix} d_{21} & d_{23} & d_{24} \\ d_{31} & d_{33} & d_{34} \\ d_{41} & d_{43} & d_{44} \end{vmatrix}$$

$$+ (-1)^{1+3} d_{13} \begin{vmatrix} d_{21} & d_{22} & d_{24} \\ d_{31} & d_{32} & d_{34} \\ d_{41} & d_{42} & d_{44} \end{vmatrix} + (-1)^{1+4} d_{14} \begin{vmatrix} d_{21} & d_{22} & d_{23} \\ d_{31} & d_{32} & d_{33} \\ d_{41} & d_{42} & d_{43} \end{vmatrix}$$

Then , we have,

$$\begin{vmatrix} d_{11} \dots d_{14} \\ . \quad . \\ d_{41} \dots d_{44} \end{vmatrix} = d_{11}d_{44}[d_{22}d_{33} - d_{32}d_{23}] + d_{11}d_{42}[d_{23}d_{34} - d_{24}d_{33}] + d_{11}d_{43}[d_{32}d_{24} - d_{22}d_{34}] -$$

$$d_{12}d_{44}[d_{21}d_{33} - d_{31}d_{23}] - d_{12}d_{41}[d_{23}d_{34} - d_{24}d_{33}] - d_{12}d_{43}[d_{31}d_{24} - d_{21}d_{34}] +$$

$$d_{13}d_{44}[d_{21}d_{32} - d_{22}d_{31}] + d_{13}d_{41}[d_{22}d_{34} - d_{32}d_{24}] + d_{13}d_{42}[d_{31}d_{24} - d_{21}d_{34}] -$$

$$d_{14}d_{43}[d_{21}d_{32} - d_{22}d_{31}] - d_{14}d_{41}[d_{22}d_{33} - d_{32}d_{23}] - d_{14}d_{42}[d_{31}d_{23} - d_{33}d_{21}] \qquad (12)$$

By using the expressions of the coefficients : d_{11} ,d_{12} , d_{13} and d_{14} which were giving in (10a) , in the expression (12) of the determinant, and after the necessary arrangement of the terms of this expression , we get the following equation :

$$\begin{vmatrix} d_{11} \dots d_{14} \\ \dots\dots.. \\ d_{41} \dots d_{44} \end{vmatrix} = (d_{22} - d_{21})[d_{33}d_{44} - d_{34}d_{43}] + (d_{41} - d_{42})[d_{33}d_{24} - d_{34}d_{23}] +$$

$$(d_{33} - d_{34})[d_{22}d_{41} - d_{21}d_{42}] + (d_{32} - d_{31})[d_{43}d_{24} - d_{44}d_{23}] +$$

$$(d_{44} - d_{43})[d_{31}d_{22} - d_{32}d_{21}] + (d_{24} - d_{23})[d_{41}d_{32} - d_{42}d_{31}] \qquad (13)$$

By the use of the expressions of the coefficients d_{ij} , which were giving in (10a) , (10b) and (a0c) , in the terms of the second member of (13) ; we get the expressions of these terms as in the following :

$[d_{33}d_{24} - d_{34}d_{23}] = [-2\beta\cosh(\beta b) + i2k\sinh(\beta b)]xe^{ikb}$

$(d_{41} - d_{42}) = i(2\alpha\cos(\alpha a) - 2ik\sin(\alpha a))xe^{-ika}$

then ,$(d_{41} - d_{42})[d_{33}d_{24} - d_{34}d_{23}] = 4i\{-\alpha\beta\cosh(\beta b)x\cos(\alpha a) + i\alpha k\cos(\alpha a)x\sinh(\beta b) + i\beta k\cosh(\beta b)x\sin(\alpha a) + k^2\sinh(\beta b)x\sin(\alpha a)\}xe^{i(b-a)k}$ (14a)

$[d_{22}d_{41} - d_{21}d_{42}] = -2i(k^2 - \alpha^2)x\sin(\alpha a)xe^{-ika}$

$(d_{33} - d_{34}) = 2\sinh(\beta b)xe^{ikb}$

then,

$(d_{33} - d_{34})[d_{22}d_{41} - d_{21}d_{42}] = 4i(\alpha^2 - k^2)x\sinh(\beta b)x\sin(\alpha a)xe^{i(b-a)k}$ (14b)

$[d_{43}d_{24} - d_{44}d_{23}] = 2(\beta^2 + k^2)x\sinh(\beta b)xe^{ikb}$

$(d_{32} - d_{31}) = -i2\sin(\alpha a)xe^{-ika}$

then,

$(d_{32} - d_{31})[d_{43}d_{24} - d_{44}d_{23}] = -4i(\beta^2 + k^2)x\sinh(\beta b)x\sin(\alpha a)xe^{i(b-a)k}$ (14c)

$[d_{31}d_{22} - d_{32}d_{21}] = -i2[\alpha\cos(\alpha a) + ik\sin(\alpha a)]xe^{-ika}$

$(d_{44} - d_{43}) = 2[\beta\cosh(\beta b) + ik\sinh(\beta b)]xe^{ikb}$

then,

$(d_{44} - d_{43})[d_{31}d_{22} - d_{32}d_{21}] = 4i\{-\beta\alpha\cosh(\beta b)x\cos(\alpha a) - i\beta k\cosh(\beta b)x\sin(\alpha a) - i\alpha k\sinh(\beta b)x\cos(\alpha a) + k^2\sinh(\beta b)x\sin(\alpha a)\}xe^{i(b-a)k}$ (14d)

$(d_{33}d_{44} - d_{34}d_{43}] = -2\beta xe^{i2bk}$

$(d_{22} - d_{21}) = -2\alpha i$

then,

$(d_{22} - d_{21})[d_{33}d_{44} - d_{34}d_{43}] = 4i\alpha\beta e^{2ikb}$ (14e)

and ,

$[d_{41}d_{32} - d_{42}d_{31}] = 2i\alpha e^{-2ika}$

$(d_{24} - d_{23}) = 2\beta$

Then,

$(d_{24} - d_{23})[d_{41}d_{32} - d_{42}d_{31}] = 4i\alpha\beta e^{-2iak}$ (14f)

If we make the addition of the expressions (14a) to (14f) then , we obtain the expression of the determinant (13) of the system of the four linear homogeneous equations as a function of the wave vector k . This expression is given by,

$4i\{[-2\alpha\beta\cosh(\beta b)x\cos(\alpha a)+ (\alpha^2- \beta^2) \sinh(\beta b)x\sin(\alpha a)]xe^{i(b-a)k} +\alpha\beta[e^{2ibk} + e^{-2iak}]\}$ (15)

The system (11) of the four linear homogeneous equation has a solution (on addition to the trifle solution: A = B = C = D = 0) , if the expression (15) of the determinant (13) of the coefficients d_{ij} vanishes. But, if we multiply the expression (15) by (1/i4) x exp[i(a-b)k] , this expression t remains unchanged . Then , after the multiplication of the expression (15) of the determinant (13) and make the result of the multiplication equal to zero ; and after the rearrangement of the terms of the obtained expression, we get the following condition:

$[(\beta^2- \alpha^2)/2(\alpha\beta)]x\sinh(\beta b)x\sin(\alpha a) + \cosh(\beta b)x\cos(\alpha a) = \cos[(a+b)k]$ (16)

In order to obtain a handier equation, we can represent the periodic square potential of the model by a periodic delta function , by passing to the limit where b =0 and $V_0 \longrightarrow \infty$, in such a way that the product : $(\beta^2 b/2)$ stays finite [5 ,6 7, 12 , 17] .

Then , if we set ,

$\lim(\beta^2 ab/2) = p$, (17)

$b \rightarrow 0$

$\beta^2 \rightarrow \infty$

with $(\beta^2 b/2)$ stays finite and different from zero , we obtain the handier equation :

$p[\sin(\alpha a)/(\alpha a)] + \cos(\alpha a) = \cos(ka)$ (18)

This equation is the final equation of the model of Kronig-Penney and we use this equation for our numeric study on the influence of the values of the parameter p on the widths of the firsts allowed and forbidden bands in the crystals .

Results and discussion of the numeric study on the influence of the parameter p on the widths of the bands :

In order to have wave functions of the form (3) ; in other words , for Bloch functions to exist ; the transcendental equation given by the relation (18) must have a solution for the variable $(a\alpha)$, then for the energy E of the states. As the cosine term on the right side of the equation (18) can have values only between -1 and +1 , then only those values of the parameter (αa) are allowed for which the left side falls in this range (between -1 and +1) .

Influence of the values of the parameter p on the limits of the allowed ranges of the variable $a\alpha$ for the six firsts allowed zones :

For finding the allowed ranges of the variable (αa), which are functions of the energy E of states , then of the wave vector k , we commence our study by plotting the left side of the equation (18) (the expression : $p[\sin(\alpha a)/(\alpha a)] + \cos(\alpha a)$) , as function of the variable $a\alpha$ between the values : $a\alpha = -6\pi$ and $a\alpha = +6\pi$ of this variable . The Fig.2a is plotted for $p = \pi/2$ and the figures : Fig.2b , Fig.2c ,……, and Fig.2f are plotted for the value of the parameter p equals to : π, $3\pi/2$, 2π , $5\pi/2$ and 3π respectively . The allowed values of the variable $a\alpha$ are drawn heavily on these six figures .

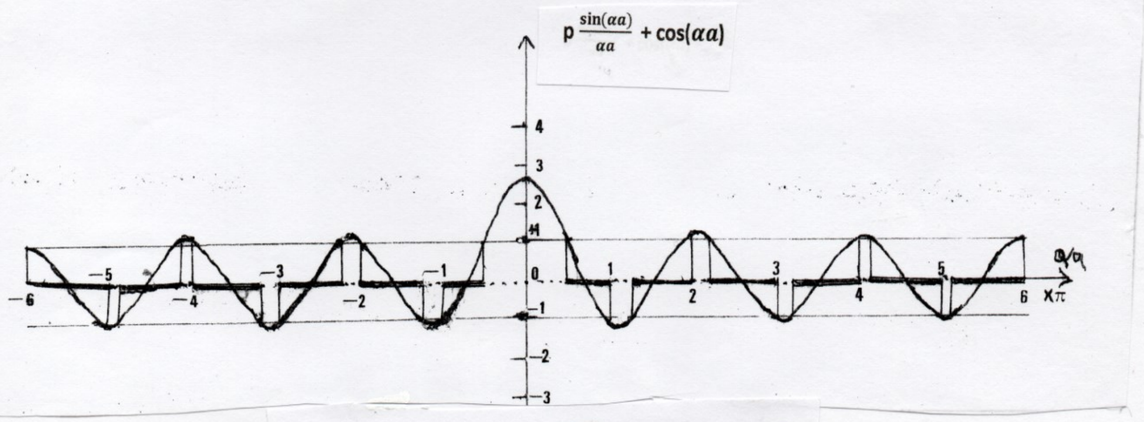

Fig.2. a Plot of the function : $p\frac{\sin(\alpha a)}{\alpha a}+\cos(\alpha a)$, for $p=\frac{\pi}{2}$

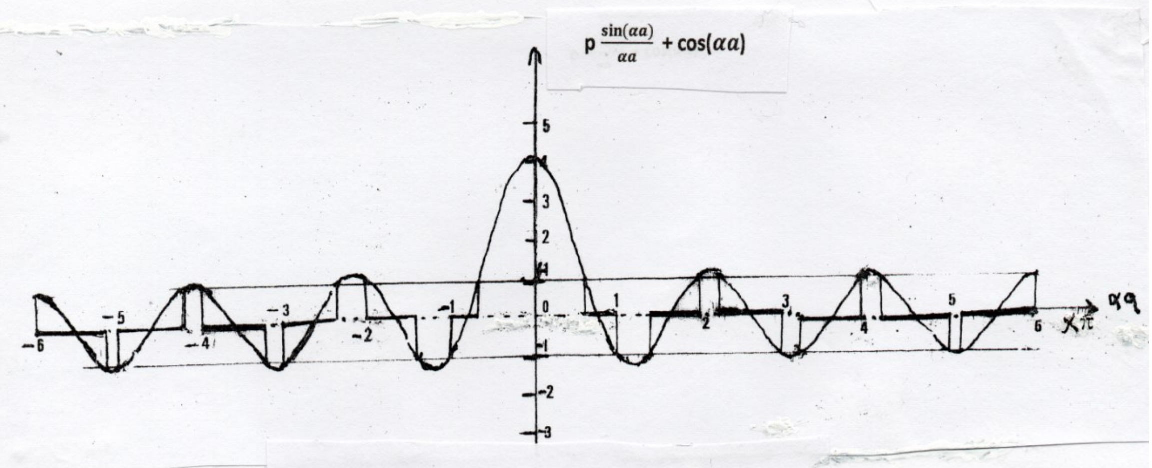

Fig.2. b Plot of the function : $p\frac{\sin(\alpha a)}{\alpha a}+\cos(\alpha a)$, for $p=\pi$

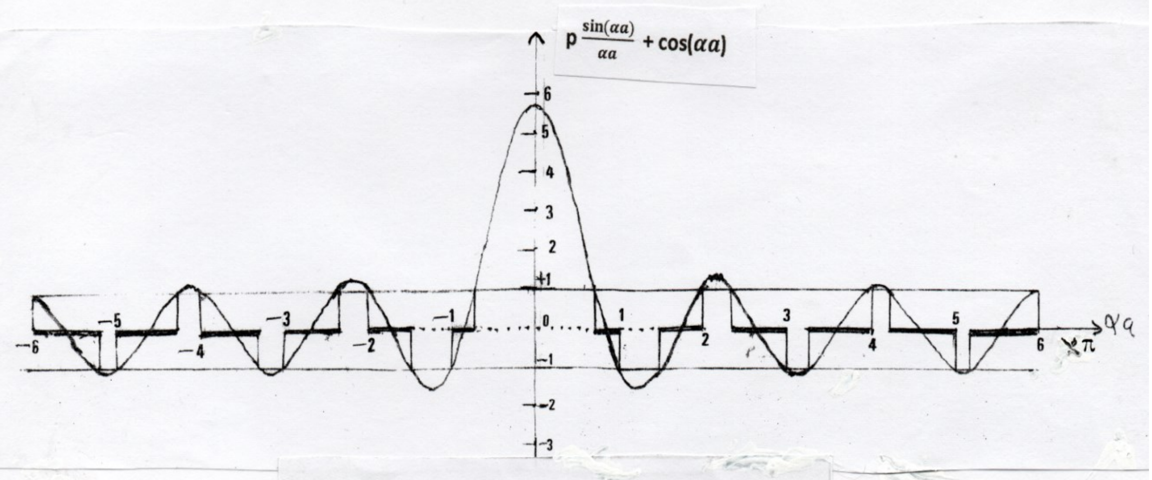

Fig.2. c Plot of the function : $p\frac{\sin(\alpha a)}{\alpha a}+\cos(\alpha a)$, for $p=\frac{3\pi}{2}$

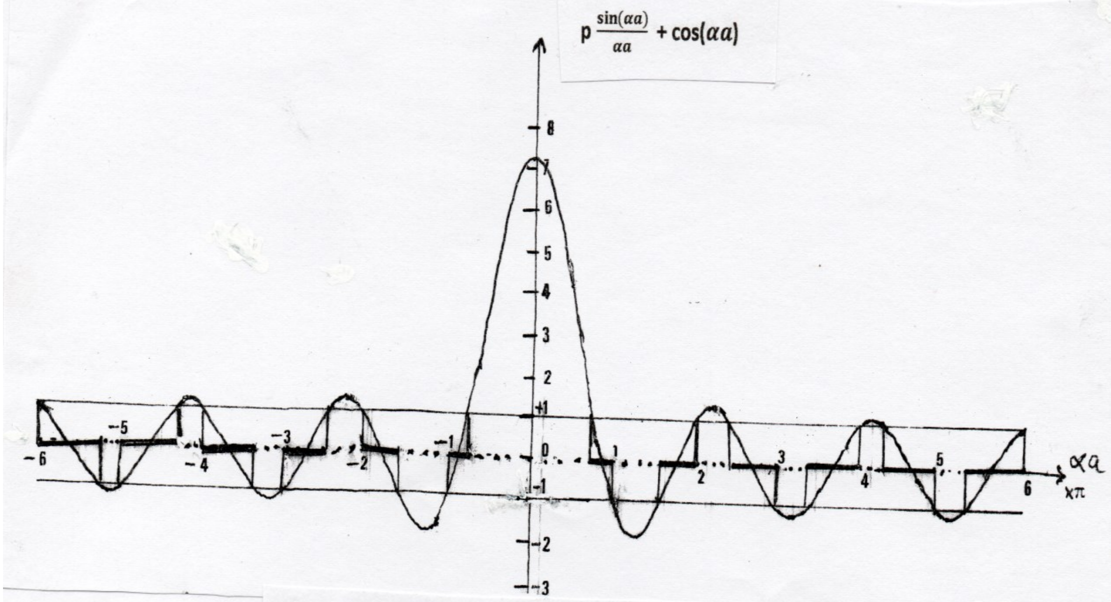

Fig.2. d Plot of the function : $p\frac{\sin(\alpha a)}{\alpha a}+\cos(\alpha a)$, for $p = 2\pi$

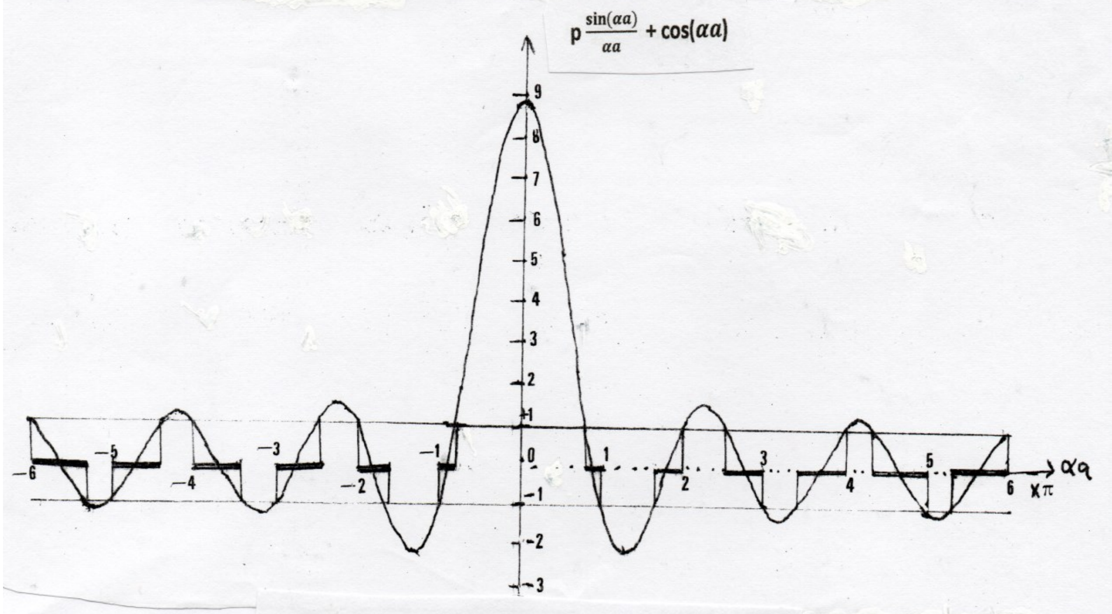

Fig.2. e Plot of the function : $p\frac{\sin(\alpha a)}{\alpha a}+\cos(\alpha a)$, for $p = \frac{5\pi}{2}$

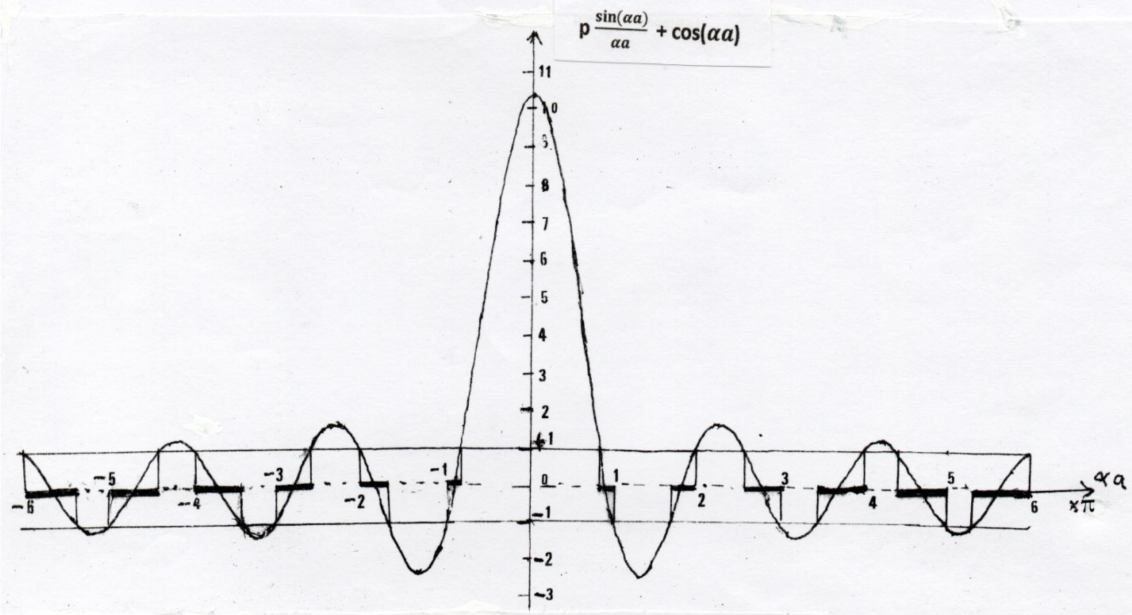

Fig.2. f Plot of the function : $p\frac{\sin(\alpha a)}{\alpha a}+\cos(\alpha a)$, for p = 3π

In the six precedent figures (the figures from the Fig.2a to the Fig.2f) one can see clearly that , with a given value of the parameter p , the upper limit of an allowed range of the parameter (aα) , which has the order n is given by nπ , where n = 1 , 2 ,3 , … Then we can always know exactly the value of the upper limit of an allowed range of αa , (then we can know exactly the value of the upper limit of the correspond allowed energy band E). The value of the lower limit of an allowed range of the parameter αa, (then the value of the lower limit of the correspond allowed energy band E) , can sometimes be know exactly and sometimes can be calculated with the tolerated percentage on the error of the calculation . In our calculation of the calculated lower limits of the allowed ranges of αa , (then of the lower limits the correspond allowed bands of E), we have always tolerated an error inferior to 0.01 per cent (0.01%) , then an error inferior to one part of ten thousand (then , our error of calculation in the following is always inferior to (1/10000).

With the help of the figures.2 ; we use the expression of the left side of the equation (18) we can determine the limits and the widths of the allowed ranges of the variable aα . Then , as given in the examples here , with the value of the parameter p equals to $\frac{\pi}{2}$: $t$he lower limit of the first allowed range of the variable αa equals to $\frac{\pi}{2}$, (for p = $\frac{\pi}{2}$ and aα = $\pi/2$ the left side of (18) gives 1) and the upper limit equals to π ; then the width of the first allowed range of the variable aα , with p = $\frac{\pi}{2}$, equals 0.5π ; while the lower limit for the second allowed range equals to 1.2434π (with this value of the variable aα , and with p = $\frac{\pi}{2}$, the left side of (18) gives -1.00000287) , and the upper limit for the second allowed range of the variable equals to 2π; then the width of the second allowed range of the variable aα equals to 0.7566π ; and the lower limit for the third allowed range of aα equals 2.1457π (with this value the left side of (18) gives 1.00003434 for p = $\frac{\pi}{2}$) and the upper limit equals to 3π ; then the width of the third allowed range of the variable aα, for p = $\frac{\pi}{2}$, equals to 0.8543π , …etc. ; we continue the calculations like this for the others allowed ranges of the variable aα with p = $\frac{\pi}{2}$; and for the others 5 allowed ranges of the variable aα with the others values of the parameter P.

In Table.1 , we collect the results of our calculations on the influence of the parameter p of the equation (18) on the limits of the allowed ranges of the variable aα for the six first allowed ranges of this variable .

Tab.1 : Influence of the values of p on the limits of the allowed ranges of $(a\alpha)$ for the sixth first allowed ranges

Value of p	Lower and upper limits	Limits of the allowed range of $a\alpha$ for the : First range	Second range	Third range	Fourth range	Fifth range	Sixth range
$\frac{\pi}{2}$	lower limit	0.5π	1.2434π	2.1457π	3.1018π	4.0777π	5.0625π
	upper limit	π	2π	3π	4π	5π	6π
π	lower limit	0.63833π	1.3958π	2.2647π	3.1933π	4.1505π	5.1226π
	upper limit	π	2π	3π	4π	5π	6π
$\frac{3\pi}{2}$	lower limit	0.71635π	1.5π	2.3604π	3.27355π	4.2175π	5.1795π
	upper limit	π	2π	3π	4π	5π	6π
2π	lower limit	0.7669π	1.57527π	2.43745π	3.3432π	4.2784π	5.23235π
	upper limit	π	2π	3π	4π	5π	6π
$\frac{5\pi}{2}$	lower limit	0.8023π	1.63183π	2.5π	3.4033π	4.3331π	5.2815π
	upper limit	π	2π	3π	4π	5π	6π
3π	lower limit	0.828465π	1.6757π	2.55133π	3.4552π	4.3822π	5.3265π
	upper limit	π	2π	3π	4π	5π	6π

From Table.1 , one can see clearly that the value of the parameter P has no influence on the values of the upper limits of the allowed ranges of the variable $a\alpha$ for every one of the allowed ranges of the variable ; while the value of the lower limit of a given allowed range of the variable $a\alpha$ increases with the increase in value of the parameter p . Then , the two limits of a given allowed range of the variable $a\alpha$ become more closer to the other when the value of p increases

Influence of the values of the parameter p on the widths of the allowed ranges and on the widths of the forbidden ranges of $a\alpha$:

By using the values in table.1, we calculate directly the widths of the first six allowed ranges of the variable $a\alpha$. We get table.2 which gives the widths of these first sec allowed range of the variable $a\alpha$ for the values of the parameter p equal to : $\pi/2$, π, $3\pi/2$, 2π , $5\pi/2$ and 3π respectively .

Tab.2 : Influence of the value of p on the widths of the allowed ranges of (αa) for the first six ranges

Value of the parameter p	Width of the allowed rang of the variable αa for the : First range	Second range	Third range	Fourth range	Fifth range	Sixth rang
$\frac{\pi}{2}$	0.5π	0.7566π	0.8543π	0.8982π	0.9223π	0.9375π
π	0.36167π	0.6042π	0.7353π	0.8067π	0.8495π	0.8774π
$\frac{3\pi}{2}$	0.28365π	0.5π	0.63961π	0.72645π	0.7825π	0.8205π
2π	0.2331π	0.42473π	0.56255π	0.6568π	0.7216π	0.76765π
$\frac{5\pi}{2}$	0.1977π	0.36817π	0.5π	0.5967π	0.6669π	0.7185π
3π	0.171535π	0.3243π	0.44867π	0.54448π	0.6178π	0.6735π

From the values of tab.1 or of Tab.2 one can see clearly that : the width of each one of the first six allowed ranges of the variable (αa) decreases with the increasing values of the parameter p , then we can expect that the width of any other allowed range of (αa) decreases with the increase in values of the parameter p ; and then the influence of the increasing values of p on the width of a given forbidden range of (αa) is completely different , because each forbidden range of the variable (αa) is between two allowed ranges . Then, the width of a given forbidden range of (αa) increases with the increase in the values of the parameter p . In reality , when the widths of two given allowed ranges decrease , the width of the forbidden range between them increases , and vice versa , when the width of a forbidden range decreases the widths of its nearby allowed ranges increase . This evident result is seen clearly with the values of the tab.2 and Tab.3 which give , respectively, the widths of the first six allowed ranges and the widths of the first five forbidden ranges of (αa) with six different values of the parameter p . We can then expect that , when the value of parameter p becomes very great , (then ,when p $\longrightarrow \infty$) , the allowed ranges of (αa) reduce to the points : nπ , (with n = $\pm$1, $\pm$2 ,$\pm$3,………) , because the lower limit of a given allowed range tends to have the value of the upper limit of this allowed ranges when the value of p becomes infinite.

Tab.3 : Influence of the value of p on the widths of the forbidden ranges of (αa) for the first five ranges

Value of the parameter p	Width of the allowed range of the variable αa for the :				
	First range	Second range	Third range	Fourth range	Fifth range
$\frac{\pi}{2}$	0.2434π	0.1457π	0.1018π	0.0777π	0.0625π
π	0.3958π	0.2647π	0.1933π	0.1505π	0.1226π
$\frac{3\pi}{2}$	0.5π	0.3604π	0.27355π	0.2175π	0.1795π
2π	0.57527π	0.43745π	0.3432π	0.2784π	0.23235π
$\frac{5\pi}{2}$	0.63183π	0.5π	0.4033π	0.3331π	0.2815π
3π	0.6757π	0.55133π	0.4552π	0.3822π	0.3265π

Influence of the value of the parameter p on the widths of the allowed energy bands:

Between the value of the parameter α and the state E of energy , we have the direct relation (7) , and this relation we get the following relation :

E = $\alpha^2\hbar^2/2$m = $4\pi^2$ ^{2} $\alpha^2\hbar^2/(8$mπ^2) = $\alpha^2 h^2$ /(8mπ^2) , (19)

But the upper limits of the allowed ranges of the parameter αa are given by the expression : α_na = nπ , n =1,2,3,..

then, by using the expression : α_n = nπ/a , n =1,2,3,.. ; in the relation (19) we get the expression of the upper limits of the allowed bands of energy E_n by the following relation :

$E_n = n^2h^2/(8ma^2)$, (20)

where the integer number n denote the order of the allowed band of energy.

For our following calculation of the widths of the allowed and forbidden bands of energy of the model , we take as unit of energy the quantity :

A $=h^2/(8a^2m_e)$, (21)

where a is the period of the linear lattice , then the period of the periodic potential.

With a = $4\text{x}10^{-10}$ m = $4\text{x}10^{-8}$cm , the value of our unity of energy equals to ;

A = $3.7653\text{x}10^{-19}$ J = 2.35 eV ,

and with a = $5\text{x}10^{-10}$ m = $5\text{x}10^{-8}$ cm, its value is :

A = $2.41\text{x}10^{-19}$ J = 1.5 eV

By using the values of the tables : Tab.1 and Tab.2 ; we give in the Tab.4 the calculated values of the widths of the first six allowed energy bands of the Kronig-Penney model ; and in the Tab.5 we give the calculated values of the widths of the first five forbidden bands between these precedent allowed bands , with an error of calculation inferior to 0.01 per cent . (0.01%) , as explained in a precedent paragraph of our study.

Tab.4 : Influence of the value of p on the widths of the allowed bands of energy E for the first six allowed bands

Value of the parameter p	Width of the allowed bands of E for the :					
	First band	Second band	Third band	Fourth band	Fifth band	Sixth band
$\frac{\pi}{2}$	0.75 A	2.45396 A	4.39597 A	6.37884 A	8.37236 A	10.37109 A
π	0.592535 A	2.05174 A	3.87113 A	5.80284 A	7.77335 A	9.75897 A
$\frac{3\pi}{2}$	0.486843 A	1.75 A	3.42851 A	5.28387 A	7.212694 A	9.17278 A
2π	0.411864 A	1.518524 A	3.05884 A	4.82301 A	6.69529 A	8.622513 A
$\frac{5\pi}{2}$	0.356315 A	1.337131 A	2.75 A	4.415749 A	6.224244 A	8.105758 A
3π	0.313646 A	1.192030 A	2.490715 A	4.0615930 A	5.796323 A	7.628398 A

Tab.5 : Influence of the value of p on the widths of the forbidden energy bands E for the five first forbidden bands

Value of the parameter p	Width of the forbidden energy band E for the :				
	First band	Second band	Third band	Fourth band	Fifth band
$\frac{\pi}{2}$	0.546044 A	0.604028 A	0.621163 A	0.627637 A	0.628906 A
π	0.948258 A	1.128866 A	1.197165 A	1.226650 A	1.241031 A
$\frac{3\pi}{2}$	1.25 A	1.571488 A	1.716130 A	1.78731 A	1.827220 A
2π	1.481476 A	1.941163 A	2.176986 A	2.304707 A	2.377487 A
$\frac{5\pi}{2}$	1.662869 A	2.25 A	2.582451 A	2.775756 A	2.894242 A
3π	1.80791 A	2.509285 A	2.93841 A	3.203677 A	3.371602 A

As examples , with a = $4x10^{-8}$ cm the width of the first allowed band passes from 1.763 eV to 1.393 eV ; when the value of p passes from $\pi/2$ to π *, and its value passes from* 1.763 *eV to* 0.968 *ev when the value of p* passes from $\pi/2$ to 2π , and the width of the fifth allowed band its width passes from 19.675 eV to 18.267 eV ; when the value of p passes from $\frac{\pi}{2}$ to π *, and its width passes from* 19.675 *eV to* 15.734 *ev when the value of p* passes from $\pi/2$ to 2π ; While , with a = $5x10^{-8}$ cm the width of the first allowed band passes from 1.125 eV to 0.889 eV ; when the value of p passes from $\pi/2$ toπ *, and its width passes from* 1.125 *eV to* 0.618 *ev when the value of p* passes from $\pi/2$ to 2π , and the width of the fifth allowed band passes from 12.559 eV to 11.660 eV ; when the value of p passes from $\frac{\pi}{2}$ to π *, and its value passes from* 12.559 *eV to* 10.043 *ev when the value of p* passes from $\pi/2$ to 2π ,
With the values of these last two tables , we see with clarity that , the width of a given allowed energy

band decreases with the increasing values of the parameter p , and on the contrary , the width of a given forbidden band increases with the increasing values of p . At the limit , when p becomes very great ($p \longrightarrow \infty$) , the allowed bands become infinitely narrow and the energy spectrum becomes a line spectrum . In reality, in that case , the equation (18) has only solutions if we have : $\sin(\alpha a) = 0$, i.e., if $\alpha a = n\pi$,with n = 1, 2, 3, 4, ….; and then , the energy spectrum is given by :

$E_n = n^2h^2/(8ma^2)$, for $p \longrightarrow \infty$

Conclusion :

In conclusion, our calculation on the influence of the parameter P of the model of Kronig-Penney on the widths of the bands of energy in the solids, revealed the following results:

1- The model shows clearly the structure of the bands for the states of energy in the solids .

2- The width of one allowed band increases with its order.

3- The increase of the value of the parameter p decreases the widths of allowed bands of energy and increases the widths of the forbidden bands of energy .

4- At the limit , when the value of p becomes infinite the spectrum of energy in the crystal becomes a line spectrum .

5- The widths of the allowed bands of energy depend grandly on the value of the parameter of crystal lattice , the width of an allowed band decreases with the increase in the value of the parameter of the lattice and the width of a forbidden band increases with the increase in the value of the parameter of the lattice.

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دراسة رقمية لتأثير قيمه البارمتر p في معادلة نموذج كرونج-بيني لحزم الطاقة على عرض هذه الحزم في الأجسام الصلبة

صالح سعيد باربيد

الملخص

في هذا البحث ، بعد أن ذكرنا بالنظرية المهمة لبلوش حول حلول معادلة شرودين جير مع الجهود الدورية ، قمنا بإثبات كيف أن البنية الدورية لآبار الجهد المربعة في بعد واحد المستخدمة في نموذج كونج – بيني لحزم الطاقة في الأجسام الصلبة تظهر بصورية جلية وواضحة بنية حزم الطاقة المسموحة والممنوعة في الأجسام الصلبة المتبلورة. وبينا أبضا كيف يتم إدخال البارامتر p في المعادلة النهائية لهذا النموذج لحزم الطاقة . ثم قمنا بدراسة رقمية وافية أظهرت كيفية تأثير هذا البارامتر في عرض (اتساع) حزم الطاقة المسموحة والممنوعة . لقد وجدنا أن عرض حزمة مسموحة ما يتقلص مع زيادة قيمة هذا البارامتر ، وعلى العكس من ذلك فإن عرض حزمة ممنوعة ما يزيد بزيادة قيمة البارامتر p .

كلمات مفتاحية : جهد دوري ، مدى مسموح ، مدى ممنوع ، منطقة (حزمة) طاقة مسموحة ، منطقة ممنوعة .