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A NUMERICAL MATRIX STUDY OF LOCALLIZED DEFECT STATES AND DIMERRIZATION IN THE ONE-DIMENSION KRONING-PENNEY MODEL

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ABSTRACT

The numerical matrix method is applied to quantum problems with periodic potentials. The numerical approaches for studying the properties of periodic potential systems, such as point defects in crystals is presented, by modifying the Kronig-Penney model, and replacing the true potential by an alternative one, and utilizing solutions to the time-independent Schrödinger equation to calculate the system' energy levels. To represent defects within crystalline systems, we modified the Kronig-Penney model—which fundamentally relies on the Marsiglio matrix approximation—and numerically simulated the matrix of periodic crystalline systems using MATLAB and Mathematic software. The problems are discrete point defects in the lattice, and dimerized Kronig – Penney mode. The obtained results showed good agreement with published values.

KEYWORDS: Kronig-Penney mdel; point defects; localized statees; energy-band gas

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NTRODUCTION

In last decade, with increasing importance of semiconductors, attention was directed toward irregular lattices. It was found that changes to the potential at a few discrete lattice sites (equivalent to lightly doped crystal) often resulted in energy levels which lay in the middle of the previously unoccupied energy gaps .It was suspected that these new states were strongly localized abo) but the irregularities that generated them (as opposed to Bloch waves which extend throughout the whole crystal[1]. Clearly important in discussion of conductivity. Somewhat later, when amorphous crystals become important, it was found that the energy level structure was maintained, but the edges of the bands were less sharply defined than previously. While these ideas are straightforward physical concepts, the mathematical complexity necessary for any kind of quantitative analytical modeling is prohibitive. Researchers in the field of crystal defects have been able to control many of the physical properties of solid materials through various defects. In ideal crystals, the atoms are arranged in a regular periodic manner without any flaw or defect. Point defects such as vacancies are simplest type of point defects in crystal, which may occur in the atomic arrangement during the crystal growth process of the material or as a result of the thermal fluctuation of the atoms around their positions in the lattice[2] . Many quanta mechanical research problems that are amenable to solution are solved using matrix mechanic[3,4]. The matrix method is especially appropriate for the potentials, it conveniently yields, with high accuracy, a whole list of eigenvalues and the associated eigenfunctions[3].

The Marsiglio matrix approach is used to study periodic potentials with the Kronig-Penney (KP) model[5], which is commonly used in solid-state physics to justify qualitatively the appearance of energy bands. This model is based on the modified free electron model and demonstrates that a simple one-dimensional periodic potential yields energy bands as well as energy band gaps[6]. We present the matrix formalism and point out its convenience for dealing with periodic potentials when a sufficiently large number of unit cells (periods) are considered. The matrix method approach provides at once numerical estimates of the first N energies and eigenfunctions of the Schrödinger equation, at the same time. [6, 7]. In this study will present the formulation of the time-independent and time- dependent Schrodinger equation[4]. Some previous studies were presented in which accurate numerical solutions were found using computer techniques for examples in one dimension, namely an infinite square well, a finite square well, and the Kronig –Penney model.[7]. We will use Mathematica & MATLAB programs to obtain accurate numerical results for some crystal defects, discrete point defects in the lattice, dimerized Kronig – Penney[8]. The aim of this work is to provide solutions to some crystal defects that are related to quantum mechanics in simple, easy and uncomplicated mathematical ways using computer techniques and programs, through which accurate numerical results were obtained[9,10].

Theoretical Framework

A. The infinite square well

In this case the particle moving under such a potential can be considered as a free particle, that means the force acting on it is zero. We do not lose generality by choosing this constant to be zero. The Hamiltonian for infinite square well potential (**box**) of width (a) is defined as:

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \qquad (1)$$

Where

$$V(x) = \begin{cases} 0 & if\ 0 \le x \le a \\ \infty & otherwise \end{cases}$$

Classically, the motion is confined to remain in the well, being maintained by repeated reflections from the walls of the well, the ψ_n vanish everywhere on the exterior of the well. We must therefore only find the interior solution for ψ_n which satisfies:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_n = E_n\,\psi_n \qquad (2)$$

And which vanishes at the boundary, $\psi_{(0)} = \psi_{(a)} = 0$. The general solution is:

$$\psi_n = A_n \sin k_n x + B_n \cos k_n x \quad , k_n = \sqrt{\frac{2mE_n}{\hbar^2}} \qquad (3)$$

Imposing the continuity condition at the origin, that is $\psi_n(0) = 0$, we find $B_n = 0$. At $x = a$ we require $\psi_n(a) = 0$ and obtain:

$$\psi_n(a) = A_n \sin k_n a = 0 \qquad (4)$$

Equation **(2)** can be solved (nontrivially, $A_n \neq 0$) only argument of the sine function is restricted to the values, $k_n a = n\pi\ ;\ (n = 1, 2, 3, \ldots)$**[3,4].**

B. The Finite symmetric well

To show how symmetry may be applied to simplify a problem, we shall consider a particle bound in a finite symmetric well**:**

$$V(x) = \begin{cases} 0 & if\ -a \le x \le a \\ V_o & otherwise \end{cases} \qquad (5)$$

If the particle has energy E, less than V_0, then according to classical mechanics the particle will be restricted to the region $-a < x < a$. The particle will be bound in this region bouncing back and forth, and any value $E > 0$ of the total energy is possible. But according to quantum mechanics only discrete values of the total energy are possible.The **Schrödinger** equation for this potential is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\,\psi(x) = E\,\psi(x) \qquad (6)$$

C. Kronig-Penney model

By merge, infinite and finite wells may form the figure of the Kronig-Penny periodic potential. A periodic potential for which the wave equation can be solved in terms of elementary functions is the square-well array. The wave equation is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_x}{dx^2} + V(x)\psi_x = E\psi_x \qquad (7)$$

Where $V(x)$ is the potential energy and E is the energy eigenvalue. In the region $0 < x < a$ in which $V = 0$, the eigenfunctions is a linear combination ,

$$\psi = Ae^{iKx} + Be^{-iKx} \qquad (8)$$

Of plane waves traveling to the right and to the left, with energy.

$$E = \hbar^2K^2/2m \qquad (9)$$

$$K^2 = 2mE/\hbar^2$$

In the region $-b < x < 0$ within the barrier the solution is of the form:

$$\psi = Ce^{Qx} + De^{-Qx} \qquad (10)$$

With $V_0 - E = \hbar^2Q^2/2m$

$$Q^2 = 2m(V_O - E)/2m \qquad (11)$$

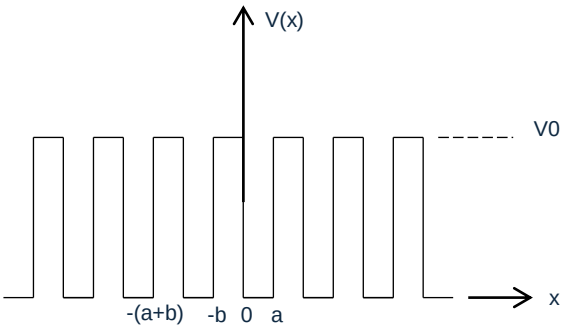


Figure (1). Square-well periodic potential as introduced by Kronig and Penney.

The complete solution to have the Bloch from **(21)** thus the solution in the region $a < x < a+b$ must be related to the solution **(10)** in the region $-b < x < 0$ by the **Bloch** theorem:

$$\psi(a < x < a + b) = \psi(-b < x < 0)e^{ik(a+b)} \quad (12)$$

Which serves to define the wavevector k used as an index to label the solution. The constant A,B,C,D are chosen so that ψ and $d\psi/dx$ are continuous at $x = 0$ and $x = a$. At $x = 0$,

$$A + B = C + D \qquad (13)$$

$$iK(A - B) = Q(C - D) \qquad (14)$$

With Q from **(10)** . At $x = a$, with the use of **(27)** for $\psi(a)$ under the barrier in terms of $(-b)$,

$$A\,e^{iKa} + Be^{-iKa} = (Ce^{-Qb} + D\,e^{Qb})e^{iK(a+b)} \quad (15)$$

$$iK(Ae^{iKa} - Be^{-iKa}) = Q\left(Ce^{-Qb} - De^{Qb}\right)e^{iK(a+b)} \quad (16)$$

The four equations **(13)** to **(16)** have a solution only if the determinant of the coefficients of A**,** B,C,D vanishes, yielding:

$$[(Q^2 - K^2)/2QK]\,sinh\,Qb\,sin\,Ka + cosh\,Qb\,cos\,Ka = cos\,k(a + b) \qquad (17)$$

The result is simplified if we represent the potential by the periodic delta function obtained when we pass to the limit $b = 0$ and $V_0 = \infty$ in such a way that $\frac{Q^2ba}{2} = P$, a finite quantity. In this limit $Q \gg K$ and $Qb \ll 1$ .Then **(17)** reduces to

$$\left(\frac{P}{Ka}\right)sin\,Ka + cosKa = cos\,ka \qquad (18)$$

The only allowed energies are those for which $-1 \leq cos\,ka \leq 1$. [5, 11,12]

D. The matrix method

A method of a numerical matrix is a practical method for quantum problems with periodic potentials, which will be used in our calculations. A matrix eigenvalue equation gives the energy levels of the periodic potential with acceptable accuracy. The methodology used to deal with problems is based on the well-known Kronig-Penney (KP) model. In addition, the Marsiglio matrix approach will be used in our calculations by implementing it in ***Mathematica and MATLAB codes***, to simulate the time-independent one-dimensional Schrodinger equation, which is given by.[7,10]

$$\hat{H}\psi_n = E_n\psi_n$$

Let H_0 be the Hamiltonian for an infinite square-well potential (box) of width L :

$$H_0 = -\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + V_{inf}(x) \qquad (19)$$

Where

$$V_{inf}(x) = \begin{cases} 0 & 0 \leq x \leq L \\ \infty & otherwise \end{cases} \qquad (20)$$

And, μ is the mass of the particle.

The eigenfunctions of H_0 are

$$\varphi_p(x) = \begin{cases} \sqrt{\frac{2}{L}}\,sin\left(\frac{p\pi x}{L}\right), & 0 \leq x \leq L \\ 0, & otherwise \end{cases} \qquad (21)$$

And the corresponding eigenvalues are

$$E_p^0 = \frac{\hbar^2\pi^2p^2}{2\mu L^2} \qquad (22)$$

With $p = 1, 2, \ldots\ldots$

Let us now denote by $\hat{H}$ the Hamiltonian of the **Schrödinger** equation:

$$\hat{H} = -\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + V(x) \qquad (23)$$

That we want to solve . Note that the potential $V(x)$ is not necessarily limited to the domain $\leq x \leq L$.
The first approximation in matrix method consist in replacing the solution of Eq.**(24)** with those of

$$H|\psi\rangle = E|\psi\rangle \qquad (25)$$

Where

$$H = H_0 + V = -\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + V_{inf}(x) + V(x) \qquad (26)$$

We will replace the infinitely repeating potential $V(x)$ with a finite periodic potential $V_{inf}(x) + V(x)$ encompassing just a few periods inside the region $0 \leq x \leq L$. Although the wave functions of the (fully) periodic $\hat{H}$ are not at all negligible outside the box, our rationale here is that the effects of the box boundaries on some quantities (e.g., the allowed energies) will be negligible if the number of periods inside the box is large enough. We will see that one can get an excellent qualitative and even quantitative description of true periodic systems by enclosing just a few periods within the box.
The next step is to note that the eigenfunctions $\varphi_p(x)$ of H_0 form a complete set of basis states for H ,so we can express any solution ψ_x of the **Schrödinger** equation (25) as the Fourier series:

$$|\psi\rangle = \sum_{m=1}^{\infty} c_m |\varphi_m\rangle \qquad (27)$$

Where c_m is a list of undetermined Fourier coefficients. Inserting Eq.(27)into **(25)**and using the orthonormality of the $\varphi_p(x)$ functions, we obtain the eigenvalue equation in matrix form:

$$\sum_{m=1}^{\infty} H_{nm}c_m = Ec_n \qquad (28)$$

Where $H_{nm} = \langle\varphi_n|H|\varphi_m\rangle$ is the nm matrix elements of H in the Fourier basis, that is:

$$H_{nm} = \delta_{nm}E_n^0 + \frac{2}{L}\int_0^L \sin(\frac{n\pi x}{L})V(x)\sin\left(\frac{m\pi x}{L}\right)dx \qquad (29)$$

With $n, m = 1, 2, \ldots$, and δ_{nm} being the Kronecker delta. Therefore, the numerical matrix method consists of

1- Embedding the potential within an infinite square well.

2- Expanding the wave function in the basis of eigenstates of the infinite square well, retaining only the first N terms of the expansion, with N chosen self consistently.

3- Solving the eigensystem, truncated at dimension N, to obtain the low-lying energies and the associated wave functions.[1, 10]

Application for Point defects

A. Discrete point defects in the lattice

We will represent the point defects by making the lattice irregular and modifying the width of one of the wells in the KP model and changing the depth of one of the wells. The effect of point defects, in the band structure of crystals can be studied by modifying some barriers in the Kronig Penney potential. We will imbed a periodic potential in an infinite square well. The Kronig-Penney potential is then

$$V_{KP}(x) = \begin{cases} 0, & |x - x_r| < b/2 \\ V_0, & otherwise \end{cases} \qquad (30)$$

Where $x_r = -\frac{a}{2} + ra$ is the position of the rth barrier, and r is an integer. Instead of using the analytical solutions, was used the matrix approach described embedding the potential within an infinite square well of width L so that the KP potential V_{KP} is replaced by

$$V_{inf}(x) + V_{KP}(x) = \begin{cases} \infty, & x \leq 0 \quad or \quad x \geq L \\ V_0, & |x - x_r| < b/2 \\ 0, & otherwise \end{cases} \qquad (31)$$

Where $r = 1, \ldots\ldots, n_b$, with $n_b = \frac{L}{a}$ the number of barriers, b is width centered barrier in each unit cell.

The matrix elements $H_{nm} = H_{nm}^{KP}$

$$H_{nm}^{KP} = E_n^{(0)}\delta_{nm} + V_0\sum_{r=1}^{nb} h_{nm}(x_r, b) \qquad (32)$$

With n, m =*1,2,…..* and δ_{nm} being the Kronecker delta.

$$h_{nm}(s, b) = \frac{2}{L}\int_{s-b/2}^{s+b/2} \sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{m\pi x}{a}\right)dx \qquad (33)$$

This integration can be solved using trigonometric identities to obtain:

$$h_{nm}(s, b) = F_{nm}(s + b/2) - F_{nm}(s + b/2)$$

$$F_{nn}(x) = \frac{x}{L} - \frac{\sin\left(\frac{2\pi nx}{L}\right)}{2\pi n} \quad \text{for} \quad n = m \qquad (34)$$

And

$$F_{nm}(x) = \frac{\sin[\frac{(m-n)\pi x}{L}]}{\pi(m-n)} - \frac{\sin[\frac{(m+n)\pi x}{L}]}{\pi(m+n)} \quad \text{for} \quad n \neq m \qquad (35)$$

For $n \neq m$. In what follows .We have chosen the units in such a way that $\frac{\hbar^2}{2\mu}$ and a =*1,* which means that the energies are in units of $\frac{\hbar^2}{2\mu a^2}$, μ being the mass of the particle . Functions that for a **KP** potential with lattice parameter $a = 1$ and n_b barriers:
1- Evaluate the Hamiltonian matrix H_{nm} equation (**29**).
2- Solve equation **(22)** to find the eigenenergies and eigenfunctions. The size of the system is$L = a * n_b = n_b$. The positions of the n_b barriers are stored in the vector (or list) x_rV, and the corresponding widths and heights are stored in vectors $bV$and V_0V, respectively.[7,10]

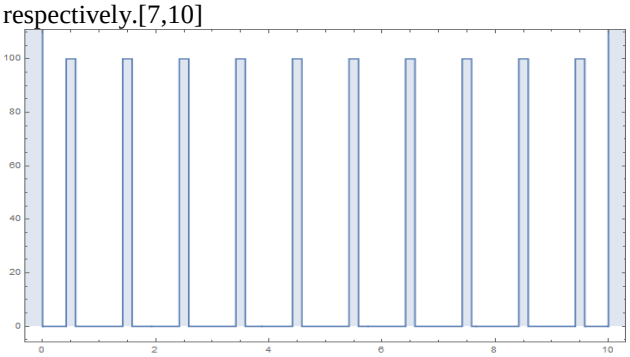


Figure (2) Show the wells original in the Kronig-Penney model.

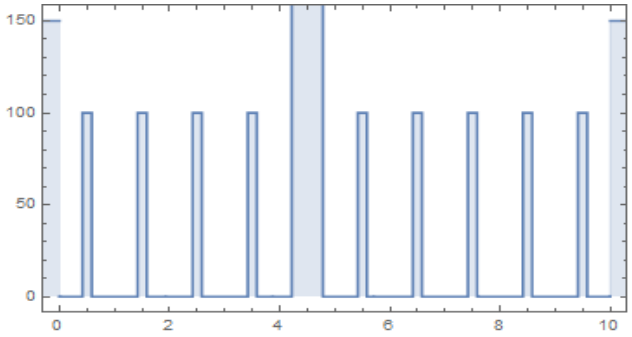


Figure.(3) Show the difference of the fifth well from the rest of the wells in the Kronig – Penny model.

Next, we generate the list of positions, widths and heights of the n_b barriers of the KP potential. While the following figure represents the calculated energies from analytical Kronig – Penney solution.

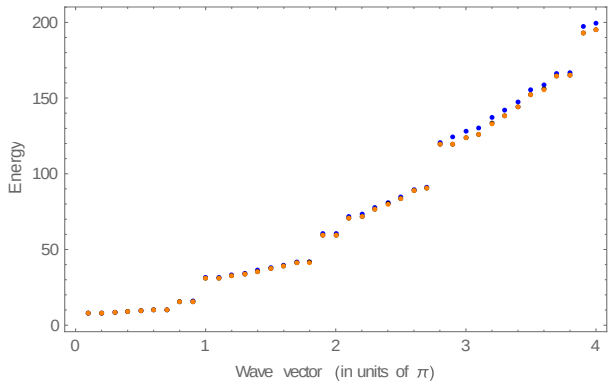


Figure (4) . Shows the energies E_n vs. kn = nπ/L , for the one - dimensional Kronig-Penney potential with barrier width $b = \frac{1}{6}$, b vector fifth3.4 b , $n_b = 10$ barriers ($l = 10$), V_0=100 and V_0vector fifth $= 3.4V_0$ calculated using the matrix method with $N = 100$.(Blue circle analytical Kronig-Penney, red circle matrix method).

Note the resonant levels within bands or localized electronic states within the forbidden energy gaps appear in this case. The continuous lines represent the energies calculated from the analytical **Kronig –Penney** solution. Our results agree with those obtained using a variant of the matrix formalism by Pavelich and Marsiglio, who make explicit use of the **Bloch** theorem to build the wave functions for the periodic **Kronig – Penney** system.

Notice that in figure (4) we plotted the energy levels vs. a scaled version of the quantum number $\boldsymbol{n}$. Using solid –state physics nomenclature, this scaled quantum number is the wave number $\boldsymbol{k_n = n\pi/L}$. It turns out that this wave number is actually related to the overall shape of the wave functions .In particular, the function $\boldsymbol{\sin n\pi x/L}$ is a good approximation for the $\boldsymbol{nth}$ state, at least away from the square-well edge; this effect is illustrated in figure (**5**) for selected values of $\boldsymbol{n}$. These are the "**Bloch standing waves**", we plotted these figures by **Mathematica**.

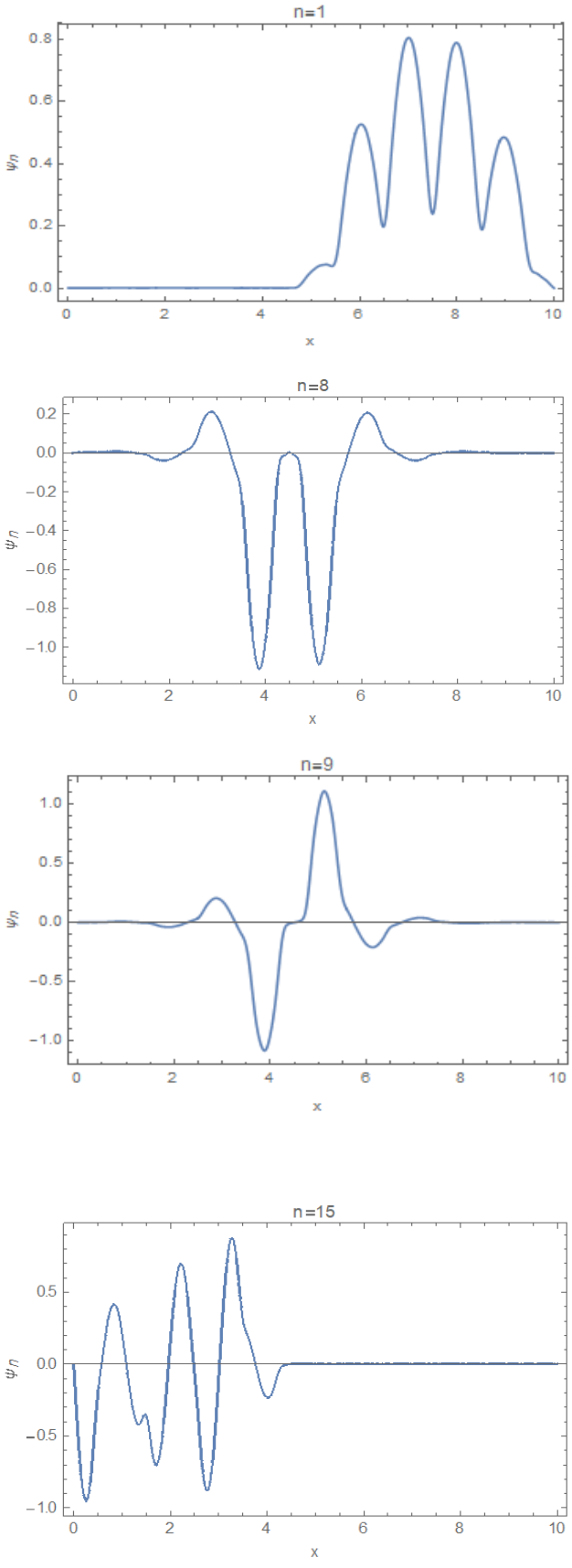


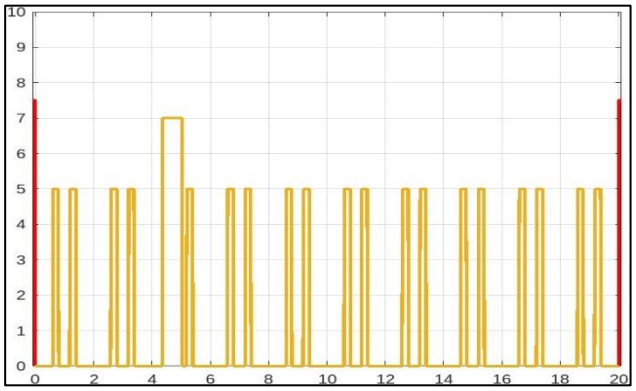
Figure (5) Eigenfunction $\psi_n(x)$ vs. x for (starting at top-left) $n = 1,\ n = 8,\ n = 9,\ n = 15$, obtained by means of the matrix method for $b = \frac{1}{6}$, b vector fifth $= 3.4\ b$,$n_b = 10$, $V_0 = 100$ and V_0 vector fifth $= 1.4V_0$ and $N = 100$, the function $0.6 \sin\left(\frac{n\pi x}{L}\right)$.

Examination of the wave function shapes shows that the presence of the impurity is very disruptive to the **Bloch** like structure of the wave functions. Some are spread throughout the lattice, others are "partitioned" by the crystal restricted either to the left of the impurity site or to the right. The exact details of the energy levels in the band and the shapes of the wave functions, are critically dependent on where the impurity was sited; and it would be expected that for a two or three dimensional lattice, any "partitioning" would not be so extreme, we notice that the wave function is biased towards the right or left side when it is in the valence band or conduction band, but when the electron is in gaps region, we notice the presence of the wave function in the middle, which enhances the conductivity of the semiconductor because when there is a defect or addition of impurity, the electron can jump from the valence band to the conduction band.

B. Dimerized Kronig – Penney

The energy spectrum of the standard Kronig - Penney model reflects mostly the of periodicity, we have to impart a livelier behavior to the latter. The simplest way of doing this is to dimerize the system as shown in figure (6) by considering a dimerized Kronig -Penney model, in which the barriers are alternately shifted right or left by a distance (u), this model is equivalent to a KP model with a unit cell of length 2 (the dimer), containing two barriers placed at locations $(1/2) + u$ and $(3/2) - u$ .The periodic potential is then $V(x) = 2P \sum_r \delta(x - x_r)$

Where $x_r = -\frac{1}{2} + r - (-1)u$ and $2P$ is parameter that determines the strength of barrier. We must employ thin , high barriers of width($b \to 0$ and $V_0 \to \infty$) with the $bV_0=2P$ held fixed that mimic Dirac delta barriers.We generate the list of positions, widths and heights of the n_b barriers of the KP potential. In this example the n_b=10 barriers have width b=1/100, b=1/10, b=1/5, b vector fifth=$3.4\ b$, height V_0=100, V_0 vector fifth=$1.4V_0$ and they are placed at the middle of each unit cell. The shift parameter is u=0.2 , N_{terms}=200.

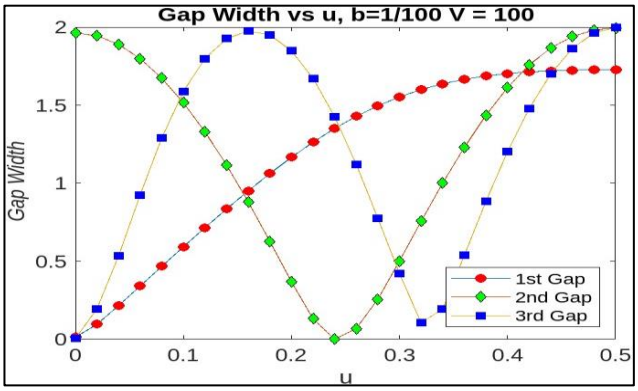


Figuer (6) Potential for the dimerized Kronig – Penney model.

Right well : dimerized potential with parameter $u \neq 0$;left well : original $u = 0$ potential. Functions that for a **KP** potential with lattice parameter $\boldsymbol{a = 1}$ and $\boldsymbol{n_b}$ barriers:

1- Evaluate the Hamiltonian matrix $\boldsymbol{H_{nm}}$ **Eq.(29).**

2- The solution of Eq.(27) The list of energies is provided directly by the function $\boldsymbol{E_n V}$. The n-th element of this matrix is the eigenvalue $\boldsymbol{E_n}$ the matrix of coefficients $\boldsymbol{c_m^{(n)}}$of Eq. **(4-10)** (28) are provided by c_n matrix. The element $(\boldsymbol{n, m})$ of this matrix is just the coefficient $\boldsymbol{c_m^{(n)}}$



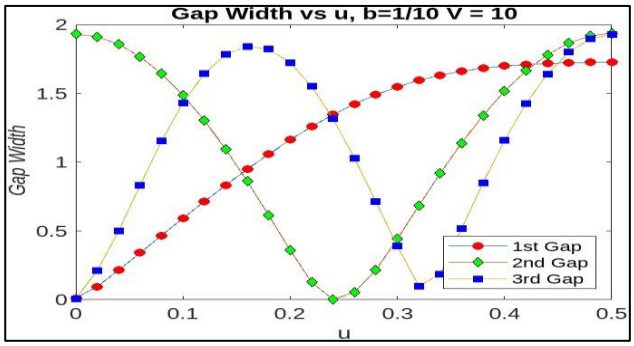
.[8]

Figure (7a)The three first gap widths vs the dimerization parameter *u* for dimerized KP model, we have used *b=1/100*, *b* vector fifth=*3.4b* , *V₀=100* and *V₀*vector fifth =1.4V₀

In the figure (7a), the red symbols a crude estimation of the first gap that appears between $\boldsymbol{n = 39n\ gap}$ and $\boldsymbol{n = 40}$ and $\boldsymbol{u = 0.2}$ The green symbols a crude estimation of the second gap that appears between $\boldsymbol{n = 79n\ gap}$ and $\boldsymbol{n = 80}$ and $\boldsymbol{u = 0.2}$. The blue symbols A crude estimation of the third gap that appears between $\boldsymbol{n = 120n\ gap}$ and $\boldsymbol{n = 121}$ and $\boldsymbol{u = 0.2}$. The improved estimation of the first gap that appears between $\boldsymbol{n = 39\ n\ gap}$ and $\boldsymbol{n = 40}$ and $\boldsymbol{u = 0.2}$,$\boldsymbol{n = 79\ n\ gap}$ and $\boldsymbol{n = 80}$ and $\boldsymbol{n = 120\ n\ gap}$ and $\boldsymbol{n = 121}$ obtained as the difference between the extrapolation

value at the middle point from the right, $E_n+1-(E_n+2-E_n+1)/2$, and from the left, $E_n-(E_n+1-E_n-1)/2$.This figure shows good agreement between the theoretical gap widths and those calculated with matrix approach.

Figure (7b) .The three first gap widths vs. the dimerization parameter u for dimerized KP model, we have used $b=1/10, b$ vectorfifth $=3.4b$, $V_0=10$ and V_0vector fifth $=1.4V_0$.



The red symbols a crude estimation of the first gap that appears between $n=39n\ gap$ and $n=40$ and $u=0.2$. The green symbols a crude estimation of the second gap that appears between $n=79n\ gap$ and $n=80$ and $u=0.2$.The blue symbols A crude estimation of the third gap that appears between $n=120n\ gap$ and $n=121$ and $u=0.2$. The improved estimation of the first gap that appears between $n=39\ n\ gap$ and $n=40$ and $u=0.2$, $n=79\ n\ gap$ and $n=80$ and $n=120\ n\ gap$ and $n=121$ obtained as the difference between the extrapolation value at the middle point from the right, $E_n+1-(E_n+2-E_n+1)/2$, and from the left, $E_n-(E_n+1-E_n-1)/2$. This figure shows good agreement between the theoretical gap widths and those calculated with matrix approach.

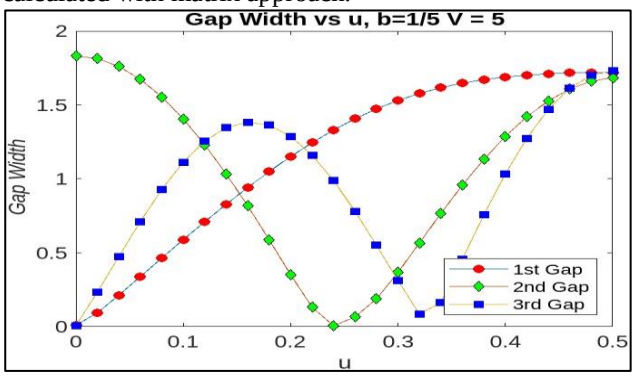


Figure (7c). The three first gap widths vs. the dimerization parameter u for dimerized KP model, we have used $b=\frac{1}{5}, b$ vector fifth $=3.4b$, $V_0=5$ and V_0vector fifth $=1.4V_0$

The red symbols a crude estimation of the first gap that appears between $n=39n\ gap$ and $n=40$ and $u=0.2$. The green symbols a crude estimation of the second gap that appears between $n=79n\ gap$ and $n=80$ and $u=0.2$. The blue symbols A crude estimation of the third gap that appears between $n=120n\ gap$ and $n=121$ and $u=0.2$. The improved estimation of the first gap that appears between $n=39\ n\ gap$ and $n=40$ for $u=0.2$, $n=79\ n\ gap$ and $n=80$ and $n=120\ n\ gap$ and $n=121$ obtained as the difference between the extrapolation value at the middle point from the right, $E_n+1-(E_n+2-E_n+1)/2$, and from the left, $E_n-(E_n+1-E_n-1)/2$. This figure shows good agreement between the theoretical gap widths and those calculated with matrix approach. Figure **(7b, 7c)** also displays the numerical results obtained with **b=1/10,V=10** ,and with **b=1/5** , **V=5**. They show that the gaps shrink as the barriers thicken. It is also notable that for relatively thick barriers with **b=1/10** the gaps are still close to those of delta –type barriers; however, the discrepancies are already important for **b=1/5**. Note finally that the differences with the behavior for delta barriers increase with the order of the gaps.

For vanishing dimerization, every odd gap vanishes (linearly with u), and none of the even ones does. The energy gaps determine the properties of solid matter, and on this basis it was classified into metals, semiconductors, and insulators, that is what the classical theory failed to do, which is neglecting the interaction of conduction electrons and periodic nature of the crystal lattice, this helps us understand electrical, thermal and optical properties of solids. In this part, the solid could have been equally well described by a unit cell containing just one delta potential. Only even gaps would have appeared, and none of them would have vanished because the transmission coefficient for one delta potential is strictly less than unity for all finite energies. We find the band structure of a dimerized Kronig-Penney model, and show its relationship to both periodicity and the transmission coefficient of the dimer, whose resonances lead to the vanishing of some of the band gaps as the dimerization varies.

CONCLUSION

Our study aimed to modified in the Kronig-Penney model, by changjng in the widths and heights well to represent ing the point defcts . Our results has carried out by using the numerical matrix procedure described by Marsiglio, the matrix method is especially appropriate for these systems because it conveniently yields, with high accuracy, a whole list of eigenvalues .This procedure has been used to show that some characteristics of fully periodic systems,In this work we have shown some important properties of crystals are controlled as much by imperfections as by the composition of the host crystal, due entirely to trace amounts of chemical imperfections. Atomic diffusion may be accelerated enormously by impurities or imperfections, and (KP)

model which demonstrates many features that are important in discussion of the point defects in materials, energy bands and impurity states. We used numerical matrix method and simple computer programming such as MATLAB & Mathematica to find all of these features in a simple, straightforward, quantitative way; but also enhances understanding of the solutions. We found that the matrix method is appropriate for these systems, because it yields, with high accuracy the energy bands, and the associated eigenfunctions. We showed some characteristics of periodic systems, such as the existence of energy bands and forbidden bands. For addition, the results showed that the band structure of a dimerized Kronig-Penney model, and show its relationship to both periodicity and the transmission coefficient of the dimer, and were our results in good agreements with the published

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