



Computation of Energy Dispersion Relation for an Electron in a one Dimensional Periodic Potential Using Intel Visual Fortran 17.0 Update 3 for Windows

Sa'adiyya, B. Bature^{1*} and Abdulqadir, M. Nura²

¹Department of Physics, Umaru Musa Yar'adua University, Katsina, Nigeria.

²Department of Physics, Bayero University Kano, Nigeria.

Authors' contributions

This work was carried out in collaboration between both authors. Author SBB performed the statistical analysis and computations, wrote the protocol, and wrote the first draft of the manuscript. Author AMN managed the analyses of the study and the literature searches. Both authors read and approved the final manuscript.

Article Information

DOI: 10.9734/ACRI/2017/37145

Editor(s):

(1) Sahaj Gandhi, Professor, Department of Physics, Bhavan'S College, Sardar Patel University, India.

Reviewers:

(1) Hulin Huang, Nanjing University of Aeronautics and Astronautics, China.

(2) S. Saravanan, Jansons Institute of Technology, India.

Complete Peer review History: <http://www.sciencedomain.org/review-history/21957>

Original Research Article

Received 2nd October 2017
Accepted 13th November 2017
Published 18th November 2017

ABSTRACT

Aims: To calculate the time independent Schrödinger's equation for an electron in a one dimensional periodic potential so as to obtain the eigenvalues of the energy.

Place and Duration of Study: Department of Physics, Bayero University Kano, Nigeria: Jan 2016 and July 2017.

Methodology: In this work, Intel Visual Fortran 17.0 update 3 for windows contained in Intel Parallel Studio XE 2017 Cluster Edition for windows was used to solve the required Schrödinger's equation with periodic potentials together with Visual Studio Community 2015 using the nearly free approximation.

Results: Here we present the Electron Energy Bands in a one dimensional periodic potential presented in a reduced zone scheme based on nearly free approximation for rectangular, sawtooth, cosine, harmonic and interpolated periodic potential. The result shows that an increase in the potential height causes an increase in the band gap and vice versa. The result shows good agreement when compared with similar results in the same model.

*Corresponding author: Email: saadiyyabature@gmail.com;

Conclusion: Our model can be used to solve the Schrödinger's equation. The energy dispersion relation for all the potentials shows that the energy gaps increases with increase in the potential where the potential was varied from 10 to 15Ry whilst keeping the spacing fixed to $a = 1.5a_0$. In Solid State Physics, a high energy gap between a filled band and an empty band corresponds to an insulator. Hence decreasing the potential height indicates that it is changing from an insulator to semiconductor.

Keywords: Nearly free approximation; one dimension; periodic potential; schrodinger equation.

1. INTRODUCTION

The differences between metals, semiconductors and insulators are explained through band theory. Electron energy levels in Solids are arranged in bands which are closely spaced energy levels approximating to a continuum. Of particular importance are the conduction band and the valence band; electrical conduction requires the presence of electrons in the upper conduction band. Between the bands are the forbidden regions or energy gaps in which no energy states are allowed. In insulators, the electron in the conduction and valence band are separated by a large energy gap, whereas in metallic conductor the conduction and valence band are very close or overlapping. In semiconductors the energy band is such as to allow movement of electrons between the valence and the conduction band under the stimulus of heat or radiation. With small gaps the introduction of foreign atoms (doping) can have a dramatic effect on electrical conductivity. An important parameter in the band theory is the Fermi level, which is the top of the available electron energy levels at low temperatures. The position of the Fermi level in relation to the conduction band is a crucial factor in determining electrical properties [1].

A particularly demanding area encountered in any course on Solid State Physics is that of the energies of electrons in crystals [2]. A peculiar aspect of the energy spectrum of an electron in a periodic potential is the presence of allowed and forbidden energy regions. One dimensional approach is particularly suited to show from different points of view (weak binding, tight binding, quantum tunneling, continued fractions) the mechanism of formation of energy bands in Solids [3]. Band structure of a material is very important to calculating the materials property, specially for obtaining the electrical properties. Usually we need to have some information about the bands to simulate electron devices [4]. An interesting phenomenon that occurs in periodic potentials, and a topic which is at the heart

semiconductor device operation, is the presence of energy bands. In many solids, there are intervals of allowed energies which particles experiencing that potential can take. That is, if one were to measure the energy of an electron in a periodic potential, they might measure values anywhere between two energies, say, a and b , but nowhere between two other energies, say c and d . The allowed energy intervals are known as energy bands and the energy difference between two bands is known as a band gap [5].

Thus, it is interesting to be able to compute the energy bands for a particular potential. Although not physically exact, the infinite periodic approximation is sufficiently good so as to provide some insight into the shape of the bands in real solids. Remarkably enough, the electronic bands in a one-dimensional system can be numerically obtained by solving an approximate eigenvalue equation. Modeling the one-dimensional case is much easier than doing it for higher dimensions, since it only allows one type of periodicity, while higher dimensions allow plenty of possible periodic lattices [6]. In many solids, such as crystals and semiconductors, atoms are arranged in an organized and periodic manner. This periodicity in the organization of the atoms leads to an electric potential that is also periodic in space. Describing the behavior of particles, such as electrons, in such potentials is a primary topic in any introductory solid state physics course, and remains an important area of research in modern electronics [7]. In the band theory framework, insulators are non-magnetic, with negligible electronic contribution C_e to the specific heat, whereas in metals, the electrons contribute a significant term linear in T which dominates at low temperatures. In addition, metals exhibit temperature-independent Pauli paramagnetism. These properties of the metal are determined by the highest energy occupied electronic states C_e , whose energy E_f defines the Fermi energy [8].

Energy dispersion relations have been investigated by several researchers using

different models. Abe (1992) calculated the energy bands of electrons in a one dimensional periodic potential consisting of multiple rectangular barriers and wells per period using transfer matrix method. The energy bands was derived from the reflection and transmission amplitudes of the individual rectangular barriers and easily extended to the cases of complex configurations of barriers and wells in the unit cell. The numerical results suggested the possibility of new type of super lattice devices composed by two different quantum wells inside the unit cell [9]. Zheng and Ando (2002) also studied the electron energy spectrum of a quantum-wire array consisting of an interface-corrugated quantum well. It is calculated for actual structures with periodic well-width variation by the [numerical diagonalization of the Hamiltonian matrix [10]. Almladh, Nelander and Pedersen (2005) illustrated the band structure concept by simulating the model systems in one and two dimensions. They used two mat-lab scripts named band. M and lab. M. The first program look at how band structure emerge in one dimension, and how it depends on the strength of the potential and separation between the ions. The reduced band scheme and meaning of reciprocal lattice were also discussed. The second program considered a two dimensional model, and the importance of potential strength was looked at and how bands overlap in the energy [11]. Fysik and Wacker (2010) considered electron in a periodic potential. The potential results both from the interaction of the electrons with ions and with other electrons, which are considered to provide a fixed background (called mean field). This entirely neglects correlations between the kinetics of the single electron and the others, and thus only serves as an approximation for the complex many Physics scenario. However, this is rather good for many purposes, in particular if more complicated potentials are used as justified within density functional theory [12]. Tanimu (2017) uses the Bloch's theorem in the absence of uniform electric field to study the electron states in a one dimensional periodic potential superimposed with an array of delta-like function. He solves the Schrodinger's equation using Newton Raphson procedure in MATLAB show how the dispersion relation changes with the energy of the particle [13].

In this research, Intel Visual Fortran 17.0 update 3 from Intel® Parallel Studio XE 2017 Cluster Edition for windows was used to solve the required Schrödinger equation with periodic

potential in connection with Visual Studio Community 2015 using the computer simulation program "Energy Bands" written by Clarke and Martin [14] edited by Boardman to obtain the energy bands in the reduced zone scheme derived from nearly free electron approximation.

1.1 Theoretical Background

The time-independent Schrödinger equation for an electron in one-dimension is

$$\left[\frac{-\hbar^2}{2m_e} \frac{d^2}{dx^2} + V(x) \right] \psi(x) = E\psi(x) \quad (1)$$

If we use the atomic units and measure energies in Rydbergs and distance in Bohr radius, then this is equivalent to setting $\hbar^2 = 1$, $m_e = 1/2$, hence for an electron equation (1) takes the form:

$$\left[\frac{-d^2}{dx^2} + V(x) \right] \psi(x) = E\psi(x) \quad (2)$$

Where $V(x)$, the potential, is periodic with period a , i.e. $V(x) = V(x+ma)$ and m is an integer.

It might appear that $\psi(x)$ should also be periodic; in fact the reality is more complicated. The probability density $\psi^*(x)\psi(x)$ is indeed periodic with period a , but this can still hold if $\psi(x)$ is equal to the product of a function which is periodic ($u(x)$ say) and a complex quantity whose product with its own complex conjugate is unity. The general form of such a complex quantity must be $\exp(i\mathbf{k}x)$, i.e.

$$\begin{aligned} \psi(x) &= \exp(i\mathbf{k}x)u(x) \text{ and} \\ \psi^*(x) &= \exp(-i\mathbf{k}x)u^*(x) \\ \psi^*(x)\psi(x) &= \exp(-i\mathbf{k}x)u^*(x)\exp(i\mathbf{k}x)u(x) \\ \psi^*(x)\psi(x) &= u^*(x)u(x), \end{aligned} \quad (3)$$

It shows that the probability density is of period a . We know that for $V(x) \rightarrow 0$, the possibility suggests itself that $\exp(i\mathbf{k}x) = \exp(ikx)$ and $\psi(x) = \exp(ikx)u_k(x)$, where k subscript on $u_k(x)$ implies a dependence of the periodic function on k . Wave functions of this form are known as Bloch functions. (Bloch first established this result in the present connection, on the basis of the periodic potential and ('periodic boundary condition'). One consequence of the form of the Bloch functions is that there are states at $k + \frac{2n\pi}{a}$ ($n = \pm 1, \pm 2, \dots$) with the same energy as a state at k . Consider the state $\psi_k(x) = \exp(ikx)u_k(x)$ and the state at $k' = k + \frac{2n\pi}{a}$;

$$\psi_{k'}(x) = \exp(i\mathbf{k}'x) u_{k'}(x) \quad (4)$$

$$\psi_k'(x) = \exp. (ikx)\exp\left(\frac{i2n\pi x}{a}\right)u_k'(x), \quad (5)$$

Where $\exp. \left(\frac{i2n\pi x}{a}\right)$ is of period a so that $\exp. \left(\frac{i2n\pi x}{a}\right)u_k'(x)$ is of period a . A possible form for this function, which correspond to a solution for equation (1) is

$$\exp. \left(\frac{i2n\pi x}{a}\right)u_k'(x) = u_k(x), \quad (6)$$

In which case,

$$\psi_k(x) = \psi_k'(x), \quad (7)$$

i.e. the two states are the same.

Substituting $\psi_k(x) = \exp(ikx)u_k(x)$ into equation (2) gives

$$\left[-\frac{d^2u_k(x)}{dx^2} - 2ik\frac{du_k(x)}{dx} + [k^2 + V(x)]u_k(x)\right] = Eu_k(x). \quad (8)$$

This is another form of Schrödinger's equation, in which analytical results are unobtainable, only numerical techniques can be used to achieve accurate results.

However, there are three entirely equivalent ways in which the E-k relationship can be presented, i.e.

- (a) The extended zone scheme, in which E is a single-valued function of k and all the relevant Brillouin zones are shown.
- (b) The reduced zone scheme, in which E is a multivalued function of k and only the first Brillouin zone is shown.
- (c) The repeated or periodic zone scheme, in which E is a multivalued function of k and all the relevant Brillouin zones are shown.

Furthermore, $E(k) = E(-k)$, and the electron energy depends on λ but not depend on whether the electron is traveling in the $+x$ or the $-x$ direction, so that it is only necessary to present the results for $k > 0$. In this work, and in the graphs generated by the computer program, the reduced zone scheme is used for $0 < k < \frac{\pi}{a}$ [12].

1.2 The Periodic Potential

In a real crystal a periodic potential arises from the Coulomb interaction of the electron with all of the atomic nuclei and all of the other electrons. In this program, the potential can be choose

between a number of potentials which have been selected principally with a view to their heuristic value rather than to their similarity between real crystal potentials [12]. The potentials are of period 'a'. The origin is an inversion centre, i.e. $V(x) = V(-x)$ so that it is only necessary to specify them for $0 \leq (x) \leq a/2$. The potentials are:

- (i) A rectangular potential: One of the most famous potentials in theoretical mechanics, the potential is defined as

$$V(x) = \begin{cases} 0, & 0 \leq x < \left(\frac{a}{2} - \frac{b}{2}\right) \\ v_0, & \left(\frac{a}{2} - \frac{b}{2}\right) < x \leq \frac{a}{2} \end{cases}$$

Where a and b are the period and width of the potential respectively.

- (ii) A Sawtooth potential: An asymmetric potential in the shape of a sawtooth signal, defined in each lattice unit by the formula

$$V(x) = 2V_0\frac{x}{a}, 0 < x < \frac{a}{2}$$

This form is used so that $V(x=a/2) = V_0$.

- (iii) A cosine potential: The most simple potential, it has only one Fourier coefficient. The frequency of the potential coincides with that of the spatial lattice, so it repeats after a distance a ($= 1$ as our unit of length)

$$V(x) = V_0\{1 - \cos\left(\frac{2\pi x}{a}\right)\}.$$

- (iv) A harmonic potential: This is a periodic potential that is proportional to x -squared. The potential is defined as

$$V(x) = 4V_0\frac{x^2}{a^2}, 0 < x < \frac{a}{2}$$

So that again $V(x = a/2) = V_0$.

- (v) Finally, an arbitrary potential can be set up by linear interpolation specifying the number of points, their x -values and the potential at each point.

1.3 The Nearly Free Electron Approximation

The opposite extreme of very low values of V_0 can be treated using the nearly-free approximation. If $V(x) = 0$, then $\psi(x) = \exp(ikx)$

and $E = k^2$. If $V(x)$ is small we can treat it as a perturbation and from the usual expression for non-degenerate perturbation theory, up to second order,

$$\begin{aligned}
 E &= k^2 + \frac{1}{a} \int_0^a \psi_k^*(x) V(x) \psi(x) dx \\
 &\quad + \frac{1}{a^2} \int_{-\infty}^{+\infty} \frac{|\int_0^a \psi_{k'}^*(x) V(x) \psi_k dx|^2 dk'}{(k^2 - k'^2)} \\
 &= k^2 + \frac{1}{a} \int_0^a \exp(-ikx) \sum_{i=-N}^{+N} f_i \exp\left(\frac{i2\pi jx}{a}\right) \exp(ikx) dx \\
 &\quad + \frac{1}{a^2} \int_{k' \neq k}^{+\infty} \frac{|\int_0^a \exp(-ik'x) \sum_{i=-N}^{+N} f_i \exp\left(\frac{i2\pi jx}{a}\right) \exp(ikx) dx|^2 dk'}{(k^2 - k'^2)} \quad (9)
 \end{aligned}$$

The factors $1/a$ and $1/a^2$ arise because the norm of the wave functions over the unit cell a . Because the exponential functions are orthogonal over the unit cell,

$$E = k^2 + f_0 + \sum_{j=-N}^{+N} \frac{f_j^2}{\left\{k^2 - \left(k - \frac{2\pi j}{a}\right)^2\right\}} \quad (10)$$

Equation (2.31) is accurate except when there is degeneracy, or near degeneracy, between the states at k and at $k - 2\pi j/a$, that is,

$$|k| \approx \left|k - \frac{2\pi j}{a}\right|, \quad (j \neq 0) \quad (11)$$

Leading to

$$k \approx -k + \frac{2\pi j}{a}, \quad (12)$$

It implies that

$$k \approx \frac{\pi j}{a} \quad (j = \pm 1, \pm 2, \dots), \quad (13)$$

As will be the case in the region of the zone boundaries. We then need to consider the explicit form of the wave functions which in this case all the wave functions considered are periodic just as proposed by the Bloch theorem [15].

2. MATERIALS AND METHODS

This research which is about electron energy band calculation in a one dimensional periodic potential is computational. The subroutine dsyev (double precision symmetric eigenvalues and

eigenvectors) from LAPACK 3.6 (linear algebra package) in MKL (Mathematical Kernel Library) which is inside the Intel Parallel Studio XE 2017 Cluster edition for windows together with Visual Studio 2015 Community using the Energy Band program by Clarke and Martin, in A. D. Boardman, (1980) to calculate the eigenvalues of the Hamiltonian (H). The essential materials for the research are: a laptop, windows 10 system, Intel Parallel Studio XE 2017 cluster edition for windows, Visual Studio 2015 Community and the subroutine dsyev from LAPACK in MKL.

The program "Energy Bands" from Physics program [12] was modified by replacing the NAG subroutine with DSYEV from LAPACK in MKL and used to calculate the first three energy levels for an electron subject to a given periodic potential. The program was used to choose the potential from the set of given periodic functions described in section 1.2 above. The type of potential was selected (NPOT) integer, the height of the NPOT was then selected (V_0) as real number, the period (a) was selected as real number and lastly, the width (b) was also selected as real number. In each case, the potential was chose and the parameters were inserted up to the last potential. The graphs were plotted using Origin 5.0 because it is user friendly even though the subroutine graph was there inside the program but not used in this work.

The main program "Energy Bands" was used to calls the following subroutines in order to prepare the data for the calculations.

- Subroutine francs:

This was used to Fourier analyse the potential. For the case of all the potentials, for the purpose of obtaining the Fourier coefficients, except the interpolated potential, in which analytic expressions for the Fourier coefficients are used.

- Subroutine energy:

This subroutine is used to calculate the first three energy levels and corresponding state vectors for given k and given periodic potential.

- Subroutine dsyev:

This is used to calculates eigenvalues and optionally eigenvectors of a real symmetric matrix using double precision.

The subroutine FRANCS (NTERMS, NDATA, DC, A) was called to find the coefficients of the cosine terms in the Fourier series, next the subroutine ENERGY was modified to be the subroutine ENERGY (K, E, EV,ND, N, LWORK, WORK, DC, A, H) so as to be to call DSYEV to calculates the energy eigenvalues and eigenvectors. Lastly, the subroutine DSYEV (S, T, N, H, ND, E, WORK, LWORK, INFO) was called within the subroutine ENERGY to calculate the eigenvalues and eigenvectors. All parameters inside each subroutine presents there meaning as used in the program.

3. RESULTS AND DISCUSSION

The program was run for rectangular, sawtooth, cosine, harmonic and the interpolated periodic potentials. A series of runs were performed, varying the chosen potential V_0 and the period a while keeping other parameters constant. The first three energy levels were computed. This describes the relationship between the energy E and the wave vector k . All inputs and outputs are in atomic units, that is the unit of distance is Bohr radius a_0 ($1 a_0 = 0.529 \text{ \AA}$) and the unit of energy is Rydberg Ry ($1 Ry = 13.6 \text{ eV}$). The energy dispersion relations were plotted.

Fig. 1 shows the energy dispersion relation for rectangular, sawtooth, cosine, harmonic and interpolated periodic potential with potential height $V_0 = 0$ and period $a = 1.5$ for the first three energy levels, with width $b = 0.5$ only when the rectangular potential is employed. It was observed that in the absence of potential there is no energy gap or band gap. Hence the presence of potential indicates the presence of band gap and vice versa. Since the potential is 0 for all the five potentials indicates that Fig. 1 represents energy dispersion relation for all the potentials since there is no potential height in each situations.

Figs. 2 – 11 shows the energy dispersion relation for rectangular, sawtooth, cosine, harmonic and interpolated periodic potentials. In which the potential was varied from 10 to 15Ry while the spacing was kept fixed to $1.5a_0$. It shows that as the potential increases, the band gap also increases and vice versa. In Solid State Physics, a high energy gap between a filled band and an empty band corresponds to an insulator. We also see that for a sufficiently high potential depth the variation of the lower bands is small compared with the energy gaps. This means that the low energy bands tend to be flatter when compared

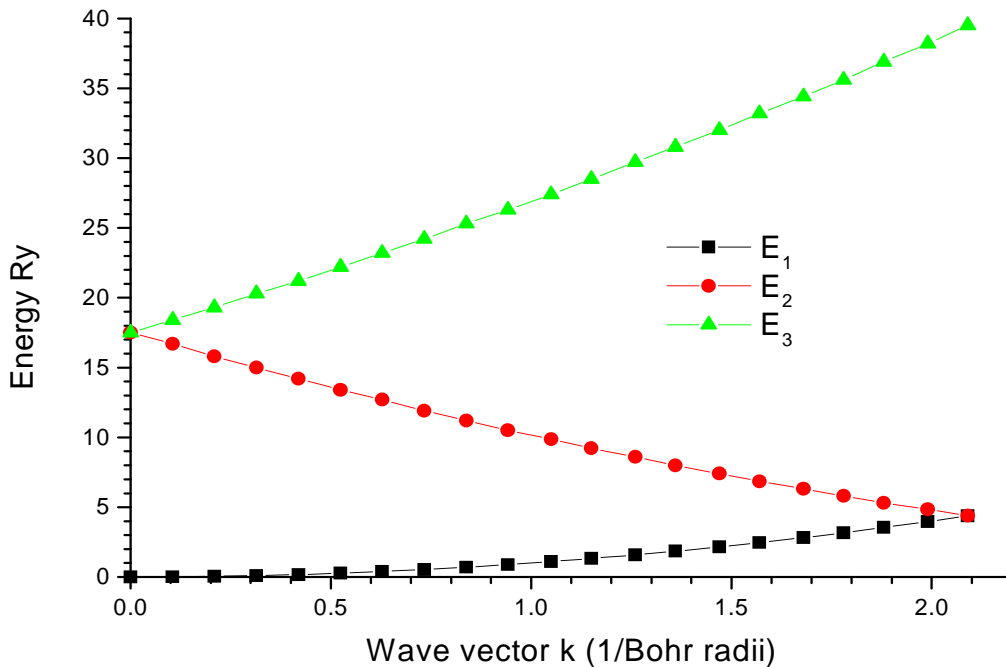


Fig. 1. E-k diagram for rectangular, Sawtooth, Cosine, Harmonic and Interpolated potentials with period $a = 1.5$, width $b = 0.5$ and potential height $V_0 = 0$ for the first three energy levels

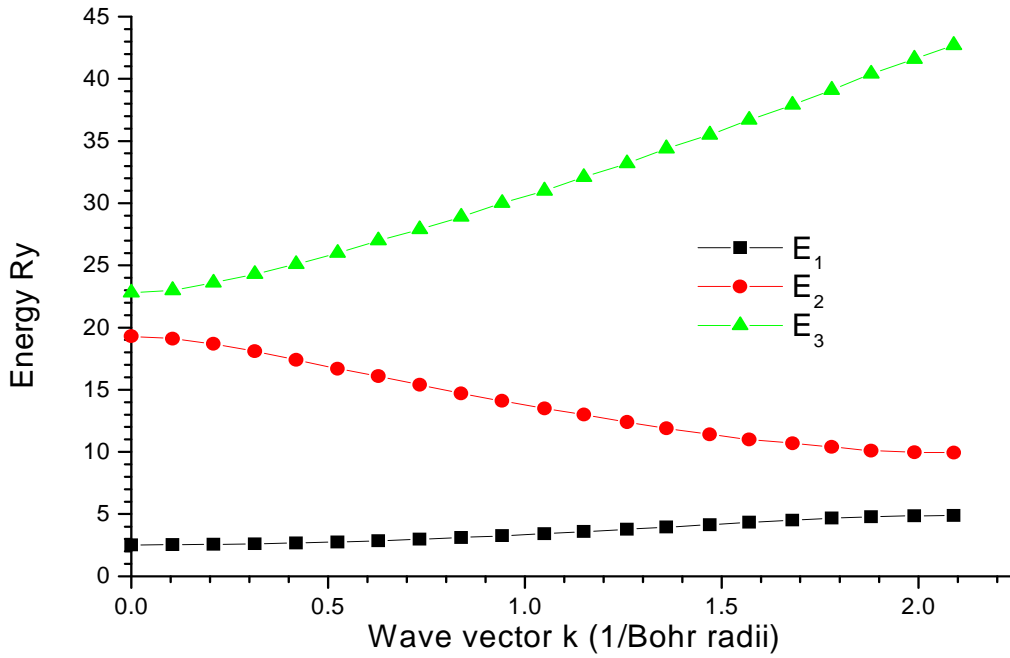


Fig. 2. E-k diagram for rectangular potential with period $a = 1.5$, width $b = 0.5$ and potential height $v_0 = 10$ for the first three energy levels

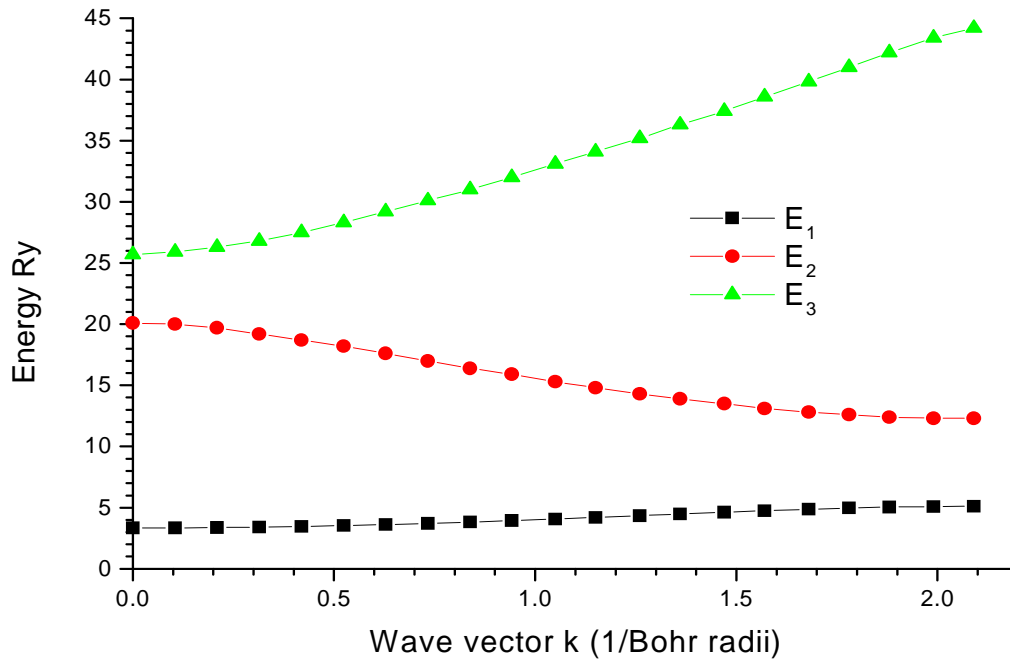


Fig. 3. E-k diagram for rectangular potential with period $a = 1.5$, width $b = 0.5$ and potential height $v_0 = 15$ for the first three energy levels

with the band separation. It is relatively simple to compare graphically the energy difference between the first and second band at $k = \pi/a$ and or between the second and third band at $k = 0$ for the cases of rectangular, cosine and harmonic potential as a function of V_0 with the

prediction of the nearly free approximation. It also shows that the presence of potential height indicates the difference in the periodic potentials,

this is so because the definition of their potentials varies for each potential as defined above in section 1.2.

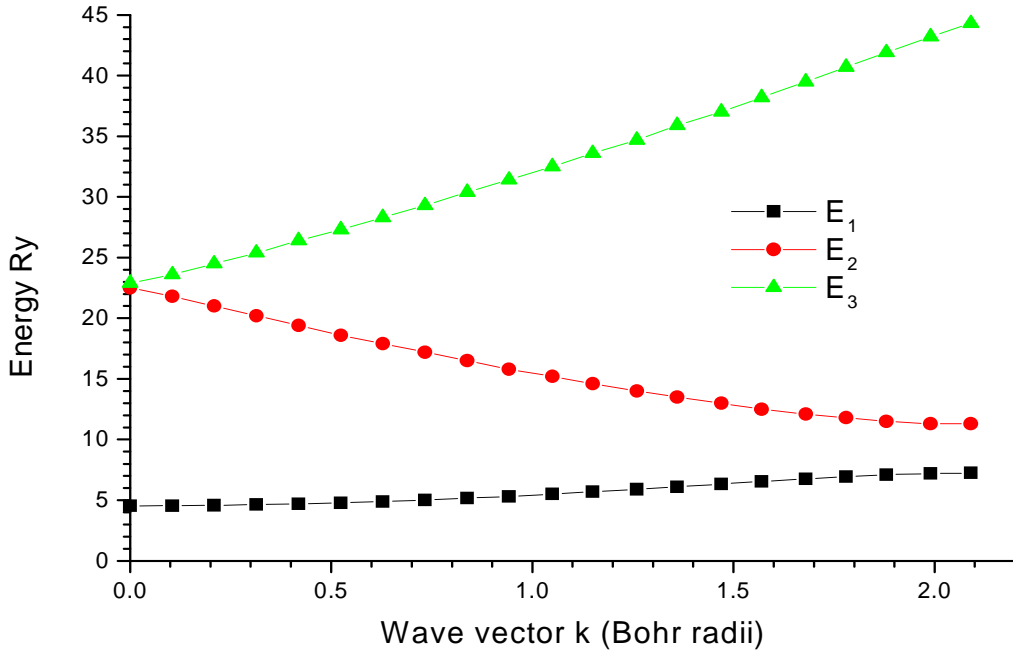


Fig. 4. E-k diagram for sawtooth potential with period $a = 1.5$ and potential height $v_0 = 10$ for the first three energy levels

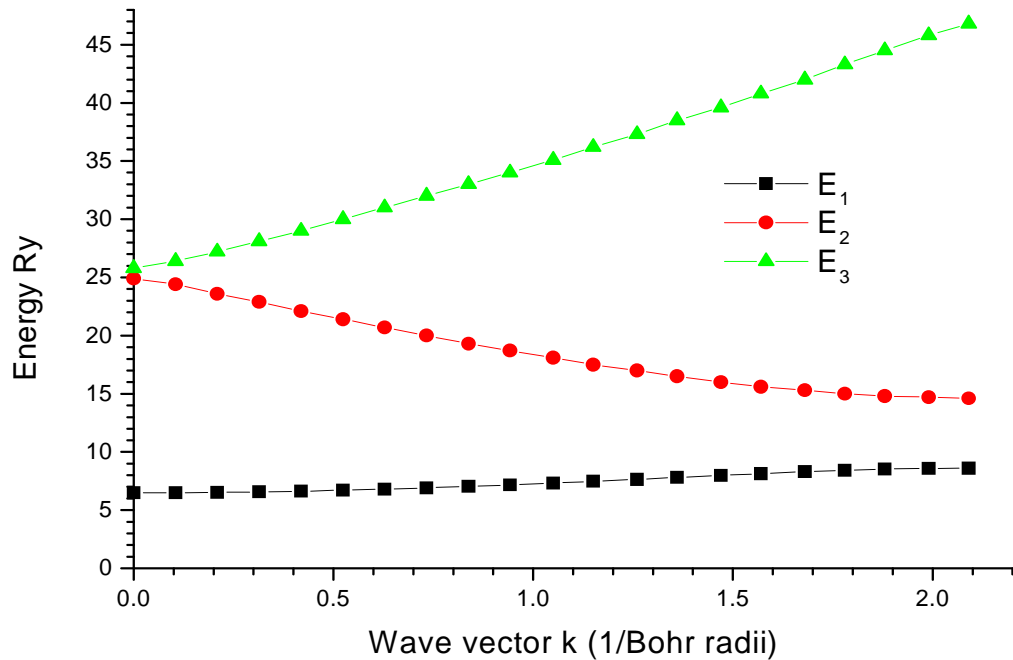


Fig. 5. E-k diagram for sawtooth potential with period $a = 1.5$ and potential height $v_0 = 15$ for the first three energy levels

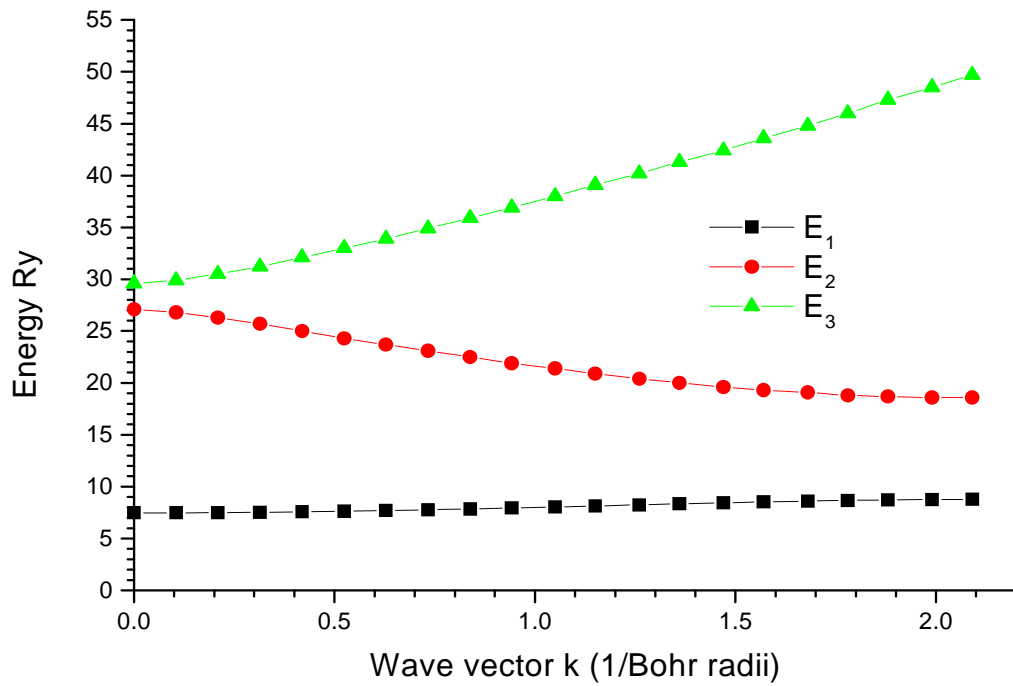


Fig. 6. E-k diagram for cosine potential with period $a = 1.5$ and potential height $v_0 = 10$ for the first three energy levels

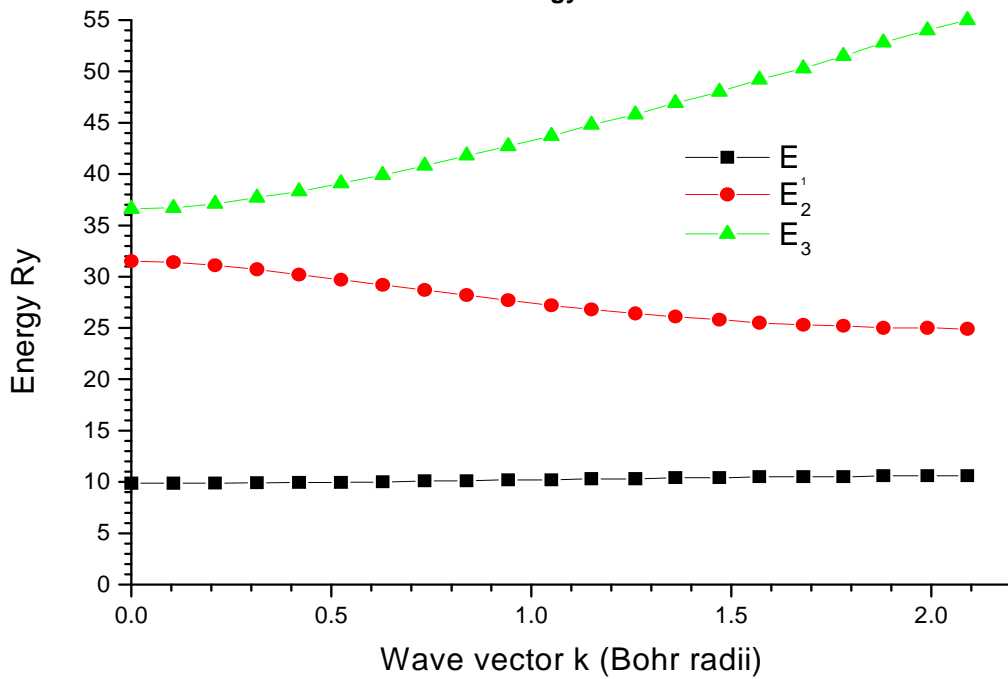


Fig. 7. E-k diagram for cosine potential with period $a = 1.5$ and potential height $v_0 = 10$ for the first three energy levels

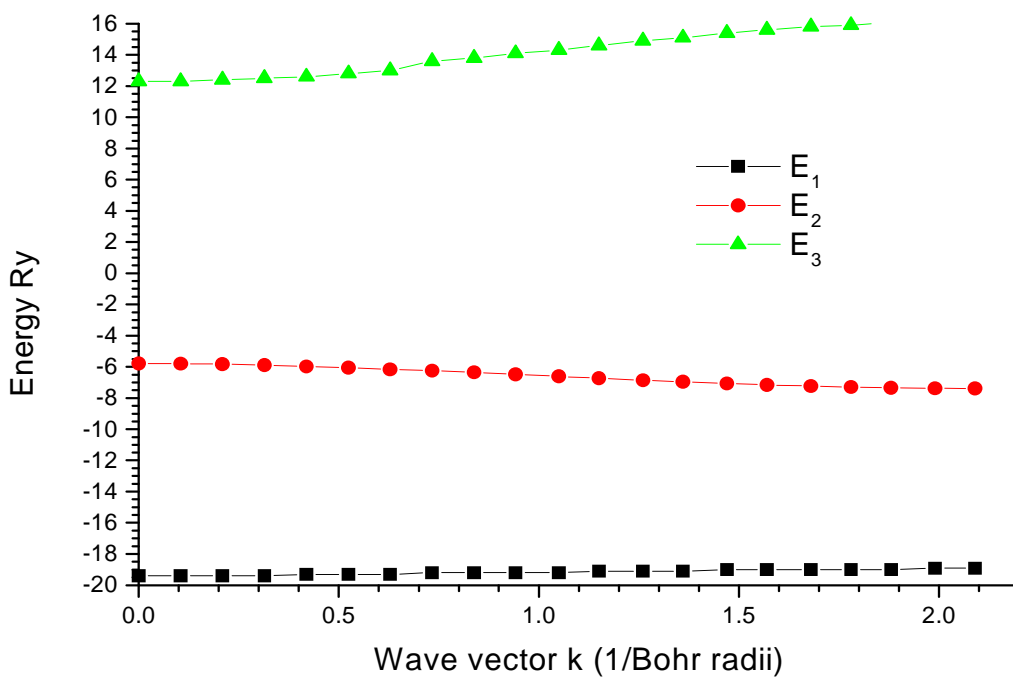


Fig. 8. E-k diagram for harmonic potential with period $a = 1.5$ and potential height $v_0 = 10$ for the first three energy levels

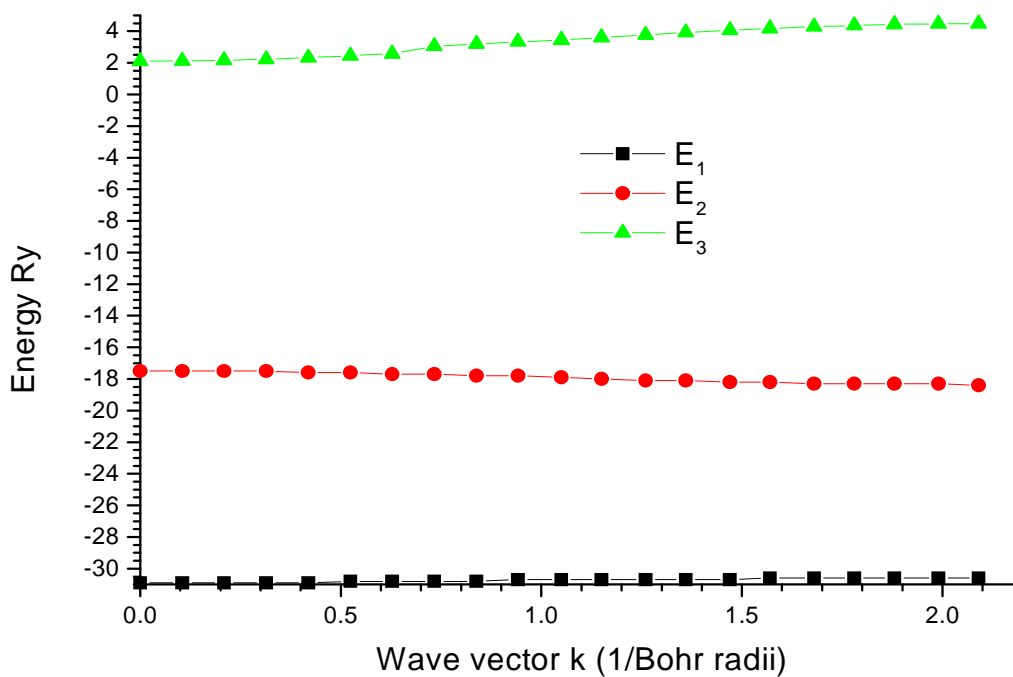


Fig. 9. E-k diagram for harmonic potential with period $a = 1.5$ and potential height $v_0 = 15$ for the first three energy levels

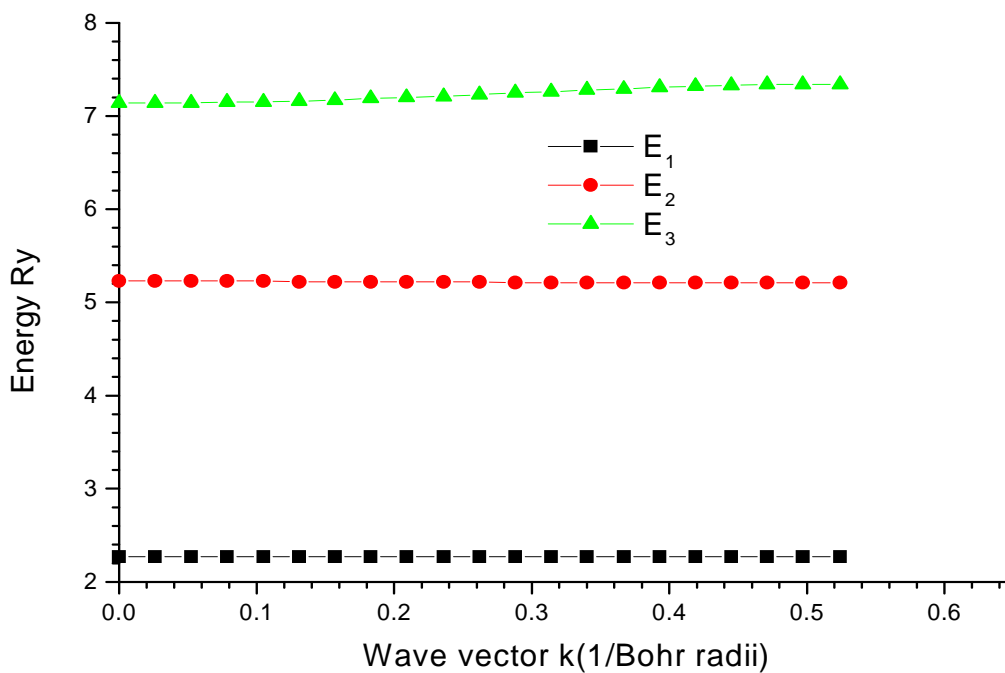


Fig. 10. E-k diagram for interpolated potential with period $a = 6.0$, number of points = 5 and potential height $v_0 = 10$ for the first three energy levels

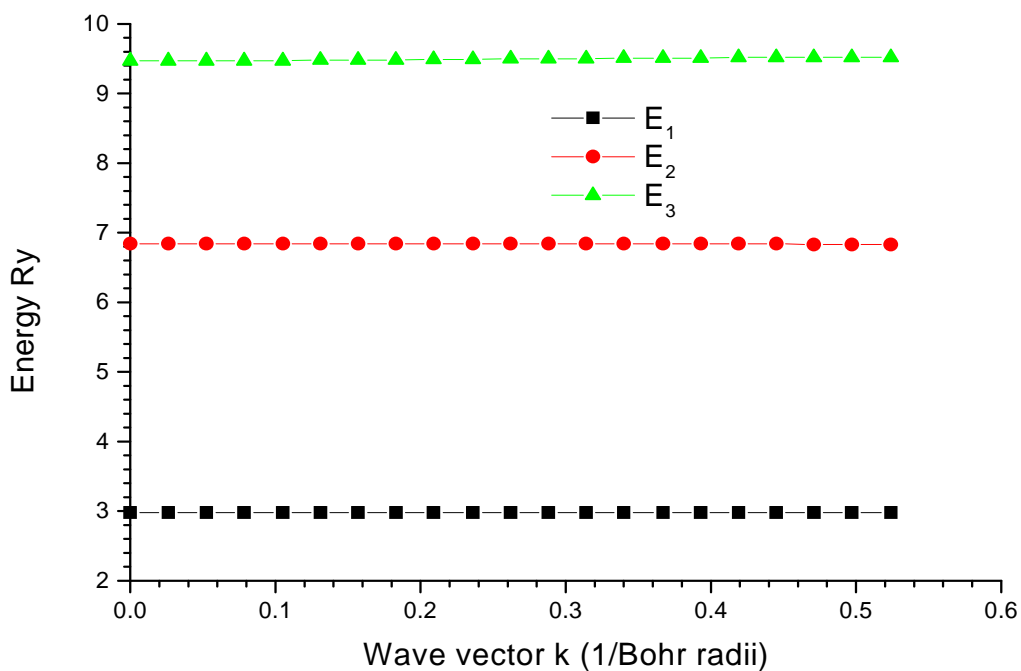


Fig. 11. E-k diagram for interpolated potential with period $a = 6.0$, number of points = 5 and potential height $v_0 = 15$ for the first three energy levels

4. CONCLUSION

In this work, the energy dispersion relation was computed for rectangular, sawtooth, cosine, harmonic and interpolated periodic potential for electron in a one dimensional periodic potential have been investigated based on nearly free electron approximation in the reduced zone scheme using the program "Energy Bands" from Physics program which was modified by replacing the NAG subroutines F02AAF and F02ABF with DSYEV obtained from LAPACK 3.6 which is part of the MKL in Intel Visual Fortran 17.0 update 3 for windows which is inside the Intel Parallel Studio XE 2017 Cluster Edition for Windows together with Visual Studio Community 2015. The energy dispersion relation for all the potentials shows that the energy gaps increases with increase in the potential where the potential was varied from 10 to 15Ry whilst keeping the spacing fixed to $a = 1.5a_0$. The computed results reproduced well when compared with the results of Urtiaga and Martinez, 2016.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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