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Application of the Transmission Line Method to Calculate the Energy Bands for an Electron in One Dimensional Lattice

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ABSTRACT

In this paper, we calculate the energy bands for an electron in one dimensional lattice, by solving Schrödinger equation for a periodic potential using the transmission line method. In this technique we use the impedance function, which gives information about the physics of the problem through its relation to the wave function, and from the impedance we can also compute the energy eigenvalues. Comparison of the numerical solutions obtained by the transmission line method with exact solutions and numerical solutions obtained by other methods demonstrates the accuracy of this method.

Key words: Schrödinger equation; Energy bands; Bloch's theorem.

المستخلص

في هذه الورقة تم حساب حزم الطاقة لإلكترون في شبكية في بعد واحد، وذلك بحل معادلة شرودنجر لجهد دوري باستخدام طريقة خط النقل، في هذه التقنية يتم استخدام دالة المعاوقة, والتي تعطي معلومات حول فيزياء المسألة وذلك من خلال علاقتها بالدالة الموجية, ايضا من دالة المعاوقة يمكن حساب القيم الذاتية للطاقة. من خلال مقارنة الحلول المتحصل عليها باستخدام طريقة خط النقل مع الحلول المتحصل عليها تحليليا وكذلك مع الحلول العددية المتحصل عليها بطرق عددية اخرى يتم توضيح مدى دقة هذه الطريقة.

Introduction

The Schrödinger equation for an electron moving in a potential is given by

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r}) + V(\vec{r})\Psi(\vec{r}) = E\ \Psi(\vec{r})\,. \qquad (1)$$

The potential $V(\vec{r})$ in the lattice is due to the valance electrons and the ions, because the lattice is periodic, it is natural that this potential is also periodic. Based on Bloch's theorem [1] the wave function can be written as

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$$\Psi_{\overrightarrow{K}}(\vec{r}) = e^{i\vec{K}.\vec{r}} u_{\overrightarrow{K}}(\vec{r}), \quad (2)$$

Where $u_{\overrightarrow{K}}(\vec{r})$ is also periodic.

The wave number $\overrightarrow{K}$ extends to all Brilloain zones. For each wave number $\overrightarrow{k}$ in the first Brilloain zone there should be large number of energy eigenvalues corresponding to $\vec{K} = \overrightarrow{k} + \overrightarrow{G_n}$, where $\overrightarrow{G_n}$ a reciprocal lattice vector, and n is is an integer, so the different values of $E_{\vec{k},n}$ corresponding to different bands. By applying Born-Van Karmar condition [1] in one dimension, the reciprocal lattice vector is given by

$$G_n = n\frac{2\pi}{a}, \quad (3)$$

Where a is the lattice parameter.

In addition to the introduction, this article is organized in three sections as follows: The general theory section which presents the formulation of the transmission line method; the application section, where we present a detailed description of the impedance function in order to show how we can calculate the electron energy bands by applying the resonance condition. In this section, we also briefly introduce two numerical methods to solve Schrödinger equation in one dimension for a periodic potential. One is based on perturbation theory by expanding any wave function obeying the Born-Van Karmar condition in a set of plane waves, which satisfy the boundary condition [1]. The other is based on the finite difference method, followed by displaying and discussing of the numerical results by comparing it with the results of the analytical solution. The last section is devoted to the conclusion.

General Theory

In the transmission line method [2,3] we reduce the infinite interval $-\infty < x < \infty$ to finite interval of unit single cell $0 \le x \le a$. This finite interval [0,a] is divided into mesh with $\Delta x = x_n - x_{n-1}$, then the Schrödinger equation in the interval $[x_n, x_{n+1}]$ can be written in n^{th} part of interval as

$$\frac{d^2\Psi_n(x)}{dx^2} - \gamma_n^2\Psi_n(x) = 0, \quad (4)$$

Where

$$\gamma_n = \sqrt{\frac{2m}{\hbar^2}(V_n - E)},$$

and V_n is the potential over the interval, and we can also replace it as the value of the potential at the centre of the interval $V_n = V(x_n + \Delta x/2)$, therefore γ_n is considered to be constant.

The impedance function is defined as

$$Z(x) = \frac{V(x)}{I(x)}, \quad (5)$$

Where $V(x)$ and $I(x)$ are two continuous functions defined respectively as

$$V(x) = \frac{d\Psi(x)}{dx}, \quad (6)$$

$$I(x) = -i\Psi(x). \quad (7)$$

Using Eqs. (4,6,7) we get two linear coupled first order differential equations

$$\frac{dV(x)}{dx} = i\gamma_n^2 I(x) \quad , \quad \frac{dI(x)}{dx} = -iV(x). \tag{8}$$

These two coupled first order equations can be separated as

$$\frac{d^2V}{dx^2} = \gamma_n^2 V \quad , \quad \frac{d^2I}{dx^2} = \gamma_n^2 I. \tag{9}$$

Assuming x_n is the origin point in the interval $[x_n, x_{n+1}]$, since γ_n is constant then $V(x_n)$ and $I(x_n)$ will take the two following recursion relations form

$$V(x_{n+1}) = V(x_n)cosh(\gamma_n \Delta x) + i\gamma_n I(x_n)\, sinh((\gamma_n \Delta x), \tag{10}$$

$$I(x_{n+1}) = I(x_n)cosh(\gamma_n \Delta x) + \frac{V(x_n)}{i\gamma_n} sinh((\gamma_n \Delta x). \tag{11}$$

Plug Eqs. (10,11) in Eq. (5) we get the impedance function as

$$Z(x_{n+1}) = z_n \frac{z_n tanh(\gamma_n \Delta x) - Z(x_n)}{Z(x_n) tanh(\gamma_n \Delta x) - z_n}, \tag{12}$$

where z_n is a very important quantity in the transmission line theory known as characteristic impedance which is defined as $z_n = -i\gamma_n$.

In order to calculate the eigenvalues of the system, the resonance condition of the impedance is required, this condition can be determined from Eqs. (5,6,7) as

$$\int_0^a Z(x)dx = i\, ln\left|\frac{\Psi(a)}{\Psi(0)}\right|. \tag{13}$$

We take an initial value of the energy E as a guess, when the resonance condition is satisfied. Then the guessed value of E will be the true eigenvalue of the system. It is notable that the resonance condition in Eq. (13) depends on the boundary conditions of the system. Because the main purpose of this article is to calculate the electron band diagrams in one dimensional lattice, so we have to determine the boundary condition of the system that satisfies the Bloch's theorem in one dimension which is given by the following equation,

$$\Psi(x + a) = e^{ika}\Psi(x), \tag{14}$$

where a is the lattice parameter .

Because the system is symmetric, the solution of k and $-k$ have the same energy and the general solution will be the linear combination of these two solutions which leads to a pure real solution

$$\Psi(x + a) = \Psi(x)\cos(ka). \tag{15}$$

Applications

In order to test the accuracy of the transmission line method, we apply it to two well known potentials, square well potential and delta function potential. We chose these examples because the solutions are simple and the analytic treatment is available.

i. Square Well Potential.

To describe the electron energy bands we consider a one dimensional lattice with a unit cell defined on $0 \leq x \leq a$, so the lattice parameter is a, this unit cell have a square well potential at its center is given by

$$V(x) = \begin{cases} V_0 & |x-a| \leq \frac{b}{2} \\ 0 & |x-a| > \frac{b}{2} \end{cases}, \qquad b < a \tag{16}$$

where V_0 is the energy potential height , and b is the width of the potential.

In this case, it is best to use the following boundary conditions, the initial value of the wave function as

$$\Psi(x_0) = \Psi(0) = 1.0, \tag{17}$$

Therefore the initial value of the impedance is

$$Z(x_0) = Z(0) = 0\,, \tag{18}$$

By using Bloch's theorem, we get $\Psi(a)$ as

$$\Psi(a) = \cos(ka), \tag{19}$$

Therefore the resonance condition of the impedance using Eq. (13) is

$$e^{-i\int_0^a Z(x)dx} = |\cos(ka)|. \tag{20}$$

According to Eq. (20), we can calculate the wave number k which corresponds to any given energy E provided that this energy lies in allowed band.

In Fig. 1, we show the impedance function Z(x) for an electron moving in a unit cell with a lattice parameter $a = 1\ A^0$ and having a central square well potential of width $b = 0.3\ A^0$ and energy potential height $V_0 = 100\ eV$ at an arbitrary electron energy eigenvalue $E = 23.179\ eV$, which is in the first energy band, and corresponding to the wave number $k = 0.628\ A^{0^{-1}}$ (see table 1.). The red line represents the real part of the impedance, while the blue line represents the imaginary part. It is worth noting from the figure that the real part of $Z(x)$ is equal to zero, and the imaginary part of $Z(x)$ is a piece wise smooth curve. So the numerical integral in the resonance condition is calculated using Simpson rule using two points with error of order Δx^5 by applying the following equation,

$$A_1 = \frac{\Delta x}{2}\left((Z_{n+1} + Z_n) - \frac{\Delta x}{6}(Z'_{n+1} - Z'_n)\right), \tag{21}$$

where $A_1$is the area between the impedance curve and x axis at the points x_n and x_{n+1}, and Z' is the first derivative of the impedance function.

Similarly in Fig. 2a, we show the impedance function $Z(x)$ for an electron with energy eigenvalue $E = 218.781$ eV which is in the third band and corresponding to the wave number $k = 0.628\ A^{0^{-1}}$(see table 1.). The figure shows that the imaginary part of the impedance goes to an extreme values if $\Psi(x) = 0$, thereby in the region $|Z(x_n)| < 100$ the numerical integral in the resonance condition can be calculated by Simpson rule in the form of Eq. (21) which is represented by the green area in Fig. .2b, while in the region $|Z(x_n)| \geq 100$ we modify Simpson rule by simulating the impedance function using Laurant approximation as

$$Z(x) = \frac{\mathrm{a}}{x - \mathrm{b}}, \tag{22}$$

therefore, the numerical integral is calculated by applying the following equation

$$A_2 = \frac{Z_n Z_{n+1} \Delta x}{Z_n - Z_{n+1}} \ln \left| \frac{Z_n}{Z_{n+1}} \right|, \qquad (23)$$

where A_2 is the area between the impedance curve and x axis at the points x_n and x_{n+1} represented by the grey area in Fig. 2b.

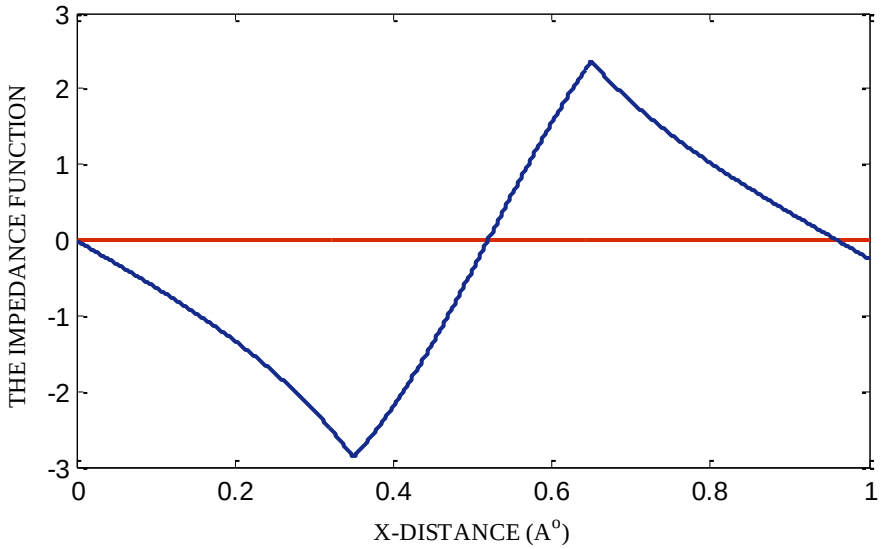

Figure 1. The impedance function for an electron in a unit cell with a=1 A^o having a central square well potential with b=0.3 A^o and V_0=100 eV at energy eigenvalue E=23.179 eV.

The imaginary part of Z(x).

The real part of Z(x).

In Fig. 3, we illustrate the electron energy bands by plotting the resonance condition of the impedance $e^{-i\int_0^a Z(x)dx}$ against the energy E for a one dimensional lattice with lattice parameter $a = 1A^0$ having a central square well potential with width $b=0.3\,A^0$ and energy potential height of $V_0 = 100\,eV$. The numerical integral is performed using mesh size of the x coordinate $\Delta x = 0.001$. In order to have a real physical running state, the value of $e^{-i\int_0^a Z(x)dx}$ must lie in the range $0 \leq e^{-\int_0^a Z(x)dx} \leq 1$, and any energy giving a value above unity lies in the band gab. In the first energy band, the value of $e^{-i\int_0^a Z(x)dx}$ decreases in the range $1 \geq e^{-i\int_0^a Z(x)dx} \geq 0$. In this range, k raises from 0 to $\frac{\pi}{2}$. Because all the values of $e^{-i\int_0^a Z(x)dx}$, are positive, it will increase again from 0 to 1 then the

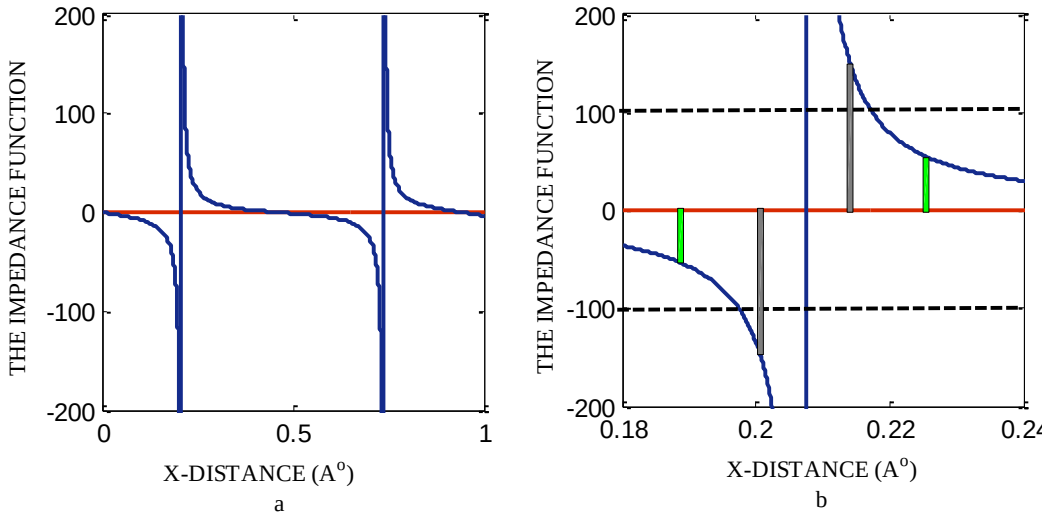

Figure 2a. The impedance function for an electron in a unit cell with a =1 A^o having a central square well potential with b =0.3 A^o and V_0=100 eV at energy eigenvalue E = 218.781 eV.

The imaginary part of Z(x).

The real part of Z(x).

Figure 2b. Illustration of the numerical integral in the resonance condition calculated by applying Simpson rule and modefied Simpson rule.

A_1 The area calculated using Eq. (21).

A_2 The area calculated using Eq. (23).

corresponding k values varying from $\frac{\pi}{2}$ to 0. So we have to shift k in this region to increase from $\frac{\pi}{2}$ to π , and in this interval an allowed energy band has appeared in which $0 \leq k \leq \pi$. In the excluded region in which $e^{-i\int_0^a Z(x)dx} > 1$ a forbidden energy band has appeared. The next allowed energy band for k starts again from 0 and increase to $\frac{\pi}{2}$ and back to 0 for values of $1 \geq e^{-i\int_0^a Z(x)dx} \geq 0$. Therefore, we have to shift k to the region $\pi \leq k \leq 2\pi$, and so on. In Fig, 3, each shaded area represents an energy band. Therefore for any given energy E we can only determine $|\cos(ka)|$ resulting in $0 \leq k \leq \frac{\pi}{2}$, so we have to shift k to the appropriate range fit to describe the band in the folded zone scheme ie, $0 \leq k \leq \pi$.

In Fig. 4, we show the first four energy bands diagram for an electron in one dimensional lattice with unit cell $a = 1A^0$ having a central square well potential with width $b = 0.3\ A^0$ and potential energy height $V_0 = 100\ eV$, calculated using the transmission line method.

In table 1, we present the first four electron energy bands corresponding to specific wave numbers k. These energy eigenvalues calculated numerically by fitting the actual results in Fig. 4, which are not regularly spaced in k- space.

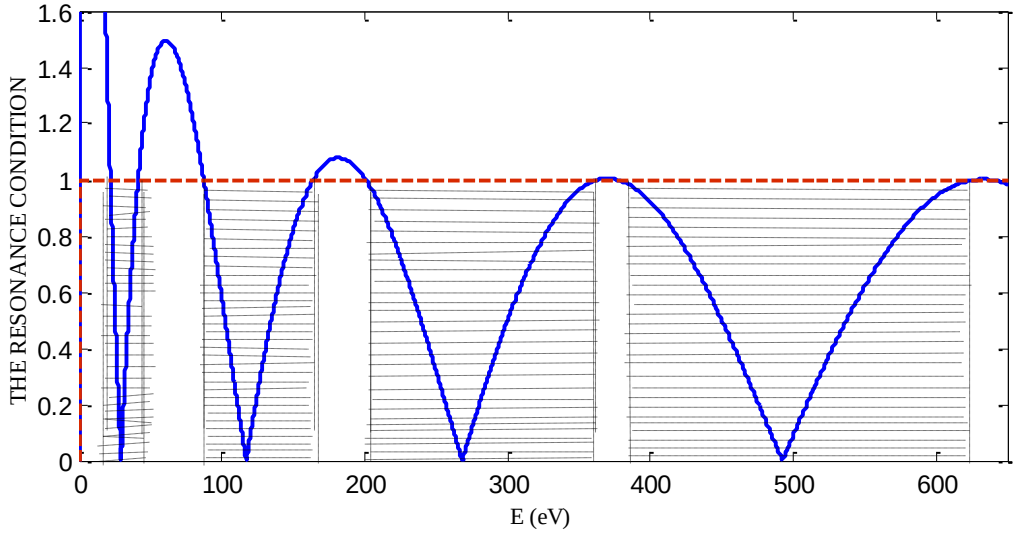

Figure 3. The resonance condition for a unit cell with a =1 A^o having a central square well potential with b =0.3 A^o and V_0=100 eV againstthe the energy.

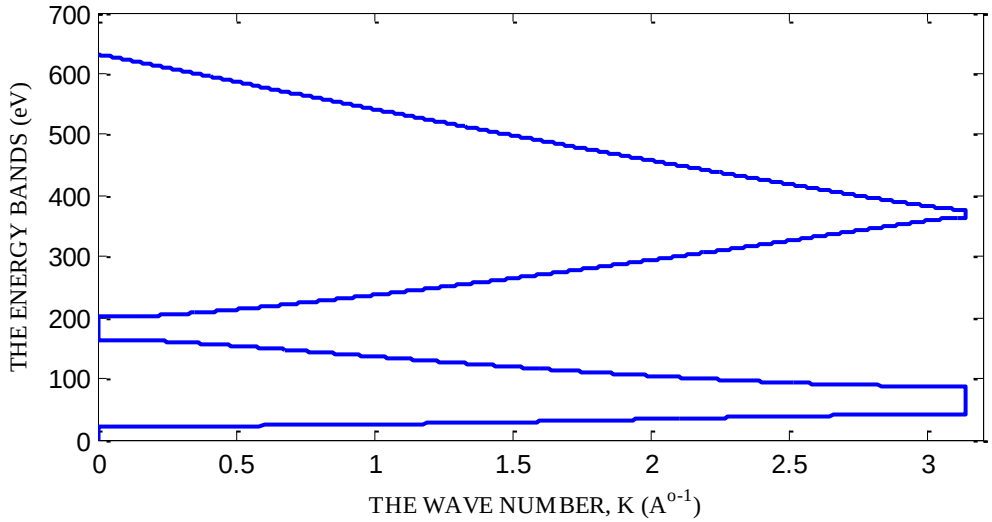

Figure 4. The first four electron energy bands in a one dimensional lattice with unit cell a =1 A^o having a central square well potential with b = 0.3 A^o and V_0 =100 eV calculated using transmission line method.

Comparison between the results obtained by applying the transmission line method and the results calculated using different methods; namely, the plane wave method, the finite difference method, and the analytic solution is illustrated in Fig. 5, as follows;

Fig.5a, for the first band, Fig. 5b, for the second band, Fig. 5c, for the third band and Fig. 5d, for the fourth band . They are in a good agreement with each other.

Table 1. The first four electron energy bands corresponding specific wave numbers k.

k (A^{o-1})	1^{st} energy band (eV)	2^{nd} energy band (eV)	3^{rd} energy band (eV)	4^{th} energy band (eV)
0	21.937	164.079	200.748	630.037
0.314	22.388	159.279	206.360	603.412
0.628	23.179	149.293	218.781	574.599
0.942	24.706	138.206	233.949	546.474
1.256	26.791	127.305	250.610	519.099
1.570	29.365	117.059	268.364	492.488
1.884	32.311	107.743	287.0456	466.652
2.199	35.422	99.633	306.565	441.611
2.513	38.351	93.114	326.836	417.4121
2.827	40.554	88.751	347.617	394.273
3.141	41.393	87.189	364.075	377.041

In the plane wave numerical method calculations, we applied the general solution for a system of m-quantum levels which is given by Schrödinger equation in the momentum domain [1]

$$\left(\mathcal{E} - \mathcal{E}^0_{k-G_n}\right)C_{k-G_n} = \sum_{n=1}^{m} U_{n-i}C_{k-G_n}, \qquad i = 1,2,\ldots\ldots m \tag{24}$$

where U_G are the Fourier coefficients which related to the periodic potential by

$$U_G = \frac{1}{all\ cell}\int dx e^{-iGx}\, V(x), \tag{25}$$

and the free electron energy $\mathcal{E}^0$ is given by

$$\mathcal{E}^0_{k-G_n} = \frac{\hbar^2}{2m}(k - G_n)^2. \tag{26}$$

In a unit cell with a lattice parameter a having a central square well potential of width b and potential energy height V_0 the Fourier coefficients are given by

$$U_G = \frac{2v_0}{a}\frac{\sin(\frac{Gfa}{2})}{G}, \tag{27}$$

where $v_0 = \frac{2m}{\hbar^2}V_0$ and $f = \frac{b}{a}$.

The results in Fig. 5, calculated by expanding the system to 100 plane waves and it involves the diagonalization of 200X200 matrix which is expensive numerically.

The results using the finite difference method [4,5] calculated numerically when $\Psi(x)$ is calculated at mesh point $x_n = n\Delta$ where $n \geq 0$, and Δ is the distance between adjacent point $\Delta = x_{n+1} - x_n$. Since $\Psi(x_n) = \Psi_n$ and to implicit fourth order in Δ,
then Ψ_{n+1} is given by;

$$\Psi_{n+1} = \frac{2 + {}^{5}/_{6}\,\Delta^2\gamma_n^2}{1 - {}^{\Delta^2}/_{12}\,\gamma_{n+1}^2}\,\Psi_n - \frac{1 - {}^{\Delta^2}/_{12}\,\gamma_{n-1}^2}{1 - {}^{\Delta^2}/_{12}\,\gamma_{n+1}^2}\,\Psi_{n-1}, \qquad (28)$$

where

$$\gamma_n = \sqrt{\frac{2m}{\hbar^2}(V_n - E)}.$$

We choose the boundary values of the wave function as following

$$\Psi(x_0) = \Psi_0 = 1.0 \quad , \quad \Psi(\Delta) = \Psi_1 = \frac{1 + {}^{5}/_{12}\Delta^2\gamma_0^2}{1 - {}^{\Delta^2}/_{12}\gamma_1^2}, \qquad (29)$$

and

$$\Psi(a) = \Psi_N = \cos(ka). \qquad (30)$$

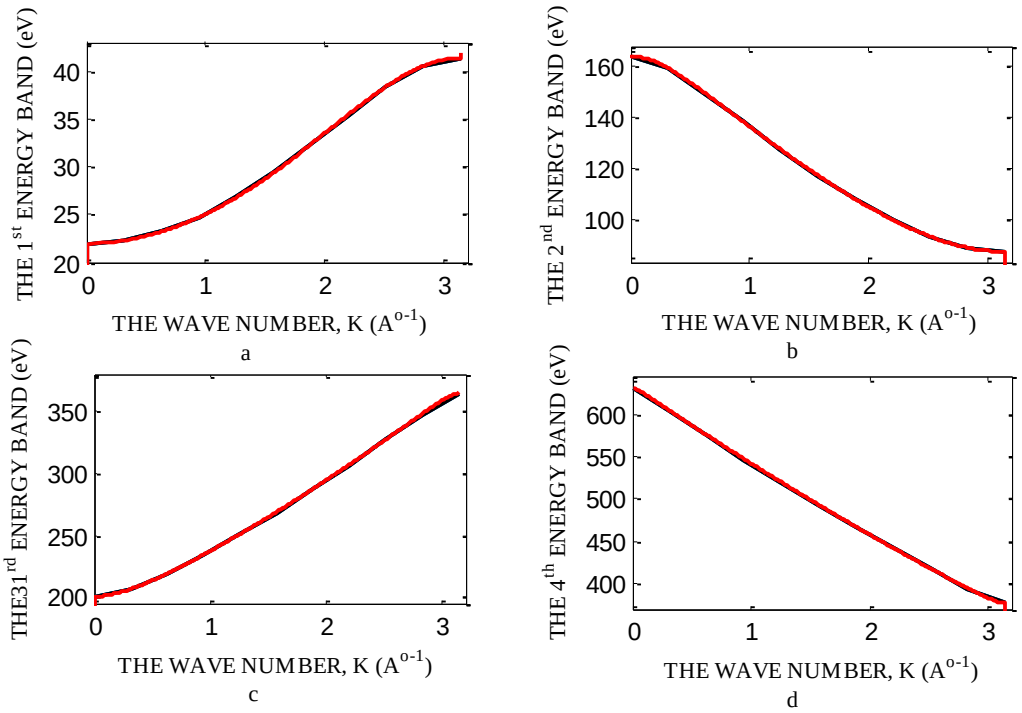

Figure 5. The first four electron energy bands in a one dimenssional lattice with unit cell a = 1 A^o having a central square well potential with b = 0.3 A^o and V_0 = 100 eV calculated using different methods.

transmission line method. finite difference method.
plane wave method. analytical solution.

For a trail value of the energy eigenvalue we calculate Ψ_N starting from Ψ_0 and Ψ_1 using Eq. (28), in this case the boundary condition is given by

$$\Psi_N = \cos(ka), \qquad (31)$$

Therefore the roots of the algebraic equation $\Psi_N - \cos(ka) = 0$ are the eigenvalues corresponding to the wave number vector which extended from 0 to π. The results in Fig. 5, calculated with $\Delta = 0.0001$ and $n = 10000$ which is also expensive numerically.

To calculate the electron energy bands illustrated in Fig. 5, analytically, we consider an arbitrary shape one bar potential $V(x)$ defined on $-\frac{a}{2} \le x \le \frac{a}{2}$ where a is a lattice parameter, to simplify we assume that the potential is symmetric $V(x) = V(-x)$ as shown in Fig. 6.

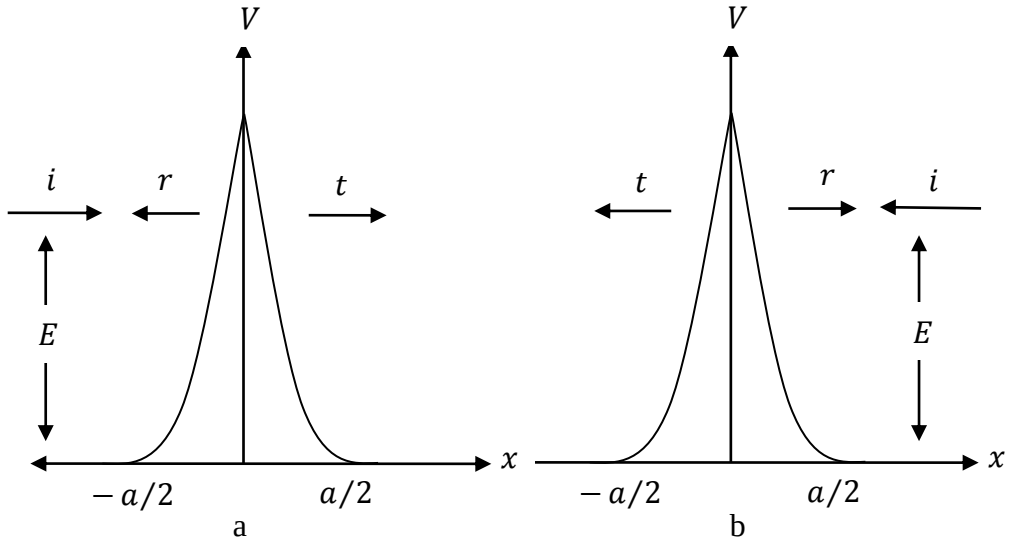

Figure 6. An arbitrary symmetric potential extending from $-a/2$ to $a/2$.
a. Represents a free electron incidents from the left side of the potential.
b. Represents a free electron incidents from the right side of the potential.

For the free electron incidents from the left side by energy given by $E = \frac{\hbar^2 K^2}{2m}$ the wave function has the following form

$$\Psi_l(x) = \begin{cases} e^{iKx} + re^{-iKx} & x \le -a/2 \\ te^{iKx} & x \ge a/2 \end{cases}, \qquad (32)$$

where r and t are the probability amplitude of the reflection and the probability amplitude of the transmission of the incident electron respectively, since the probability amplitude of the incident is the unity , so they satisfy the relation

$|t|^2 + |r|^2 = 1.$

Similarly, the wave function for a free electron with the same energy incidents from the right side can be written as

$$\Psi_r(x) = \begin{cases} te^{-iKx} & x \le -a/2 \\ e^{-iKx} + re^{iKx} & x \ge a/2 \end{cases}. \qquad (33)$$

Since Ψ_l and Ψ_r are two independent solutions for Schrödinger equation for a single potential, so the general solution is the linear combination of these two solutions

$$\Psi(x) = A\Psi_l(x) + B\Psi_r(x). \qquad -a/2 \le x \le a/2 \tag{34}$$

The solution for a one dimensional unit cell with lattice parameter can be found by applying the Bloch's theorem Eq. (15) and we get the following equation [1]

$$\cos(ka) = \frac{t^2 - r^2}{2t} e^{iKa} + \frac{1}{r^2} e^{-iKa}. \tag{35}$$

The transmission coefficient for an electron incident by energy E on a unit cell with lattice parameter a having a central square well potential of width b and potential energy height V_0 is given by [6]

$$t = \frac{4K\alpha e^{-iKf}}{4Kacos(\alpha_f) - 2i(K^2 + \alpha^2)\sin(\alpha_f)}, \tag{36}$$

and the reflection coefficient is given by

$$r = \frac{it(\alpha^2 - K^2)}{2K\alpha}\sin(\alpha_f), \tag{37}$$

where

$K = \sqrt{\frac{2m}{\hbar^2}E}$, $\alpha = \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$, and $f = \frac{b}{a}$.

ii. Delta-Function Potential.

Now we consider a one dimensional lattice with unit cell defined on $0 \le x \le a$ with central delta function potential given by

$$V(x) = V_0\delta(x - a/2), \tag{38}$$

where V_0 is the strength of the potential.

In the transmission line method, the boundary conditions and the resonance condition are very similar to those used in the case of the square well potential, represented in Eqs. (17,18,19,20), except now the impedance function given by Eq. (12) if x $\neq a/2$ while the impedance function in the position of the delta-function is given by

$$Z(x_n) = Z(x_{n-1}) + v_0 i \qquad at \qquad x = a/2 \tag{39}$$

where

$\mathcal{E} = \frac{2m}{\hbar^2}E$, $v_0 = \frac{2m}{\hbar^2}V_0$,

and Δ is the mesh size of the x coordinate.

In Fig. 7, we show the impedance function $Z(x)$ for a unit cell with a lattice parameter $a = 1A^0$ having a central delta function potential with a strength $V_0 = 100\ eV$ at arbitrary electron energy eigenvalues. In Fig. 7a, the electron energy eigenvalue $E = 29.185\ eV$ is in the first energy band and correspond to the wave number $k = 0.628\ A^{0^{-1}}$. While in Fig. 7b, the electron energy eigenvalue $E = 269.365\ eV$ is in the third energy band and correspond to the wave number $k = 0.628\ A^{0^{-1}}$. The red line represents the real part of the impedance while the blue line represents the imaginary part, the graphs show the rapidly changing of the imaginary part of the impedance at the position of delta-function. Therefore, in order to apply the resonance condition using Eq. (13) we had to calculate the numerical integral for a sufficiently small mesh size in this region.

In Fig. 8, we show the resonance condition $e^{-i\int_0^a Z(x)dx}$ against the energy E for a one dimensional lattice with lattice parameter $a = 1A^0$ having a central delta function potential with energy potential strength $V_0 = 100\ eV$. The numerical integral is performed using mesh size of the x coordinate $\Delta x = 0.0001$ at the position of delta-function.

Comparison between Fig. 3, and Fig. 8, shows that the forbidden energy bands (energy gabs) in the delta function potential are larger than those in the square well potential.

In Fig. 9, we show the first four energy bands diagram for an electron in one dimensional lattice with a unit cell $a = 1A^0$ having a central delta function potential with a strength $V_0 = 100\ eV$, calculated by the transmission line method.

The first four electron energy bands corresponding to specific wave numbers k are listed in Table 2.

The first four electron energy bands diagram are illustrate in Fig. 10, for an electron in one dimensional lattice with a unit cell $a = 1A^0$ having a central delta function potential with strength potential $V_0 = 100\ eV$. It is calculated numerically using the transmission line method, plane wave method, and finite difference method, and the analytical solution. Again, the agreement between the analytical results and those obtained numerically and the results obtained by applying the transmission line method are good.

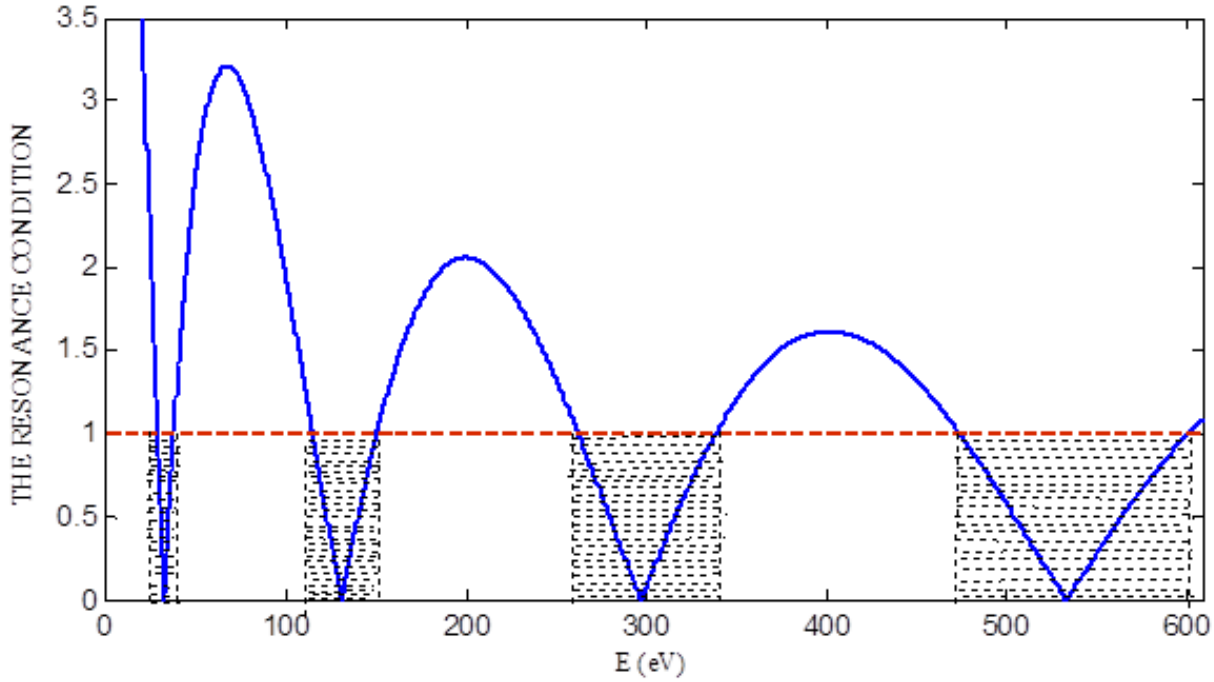

Fig. 8. The resonance condition of a unit a=1 A° having a central delta-function with V_0=100 eV against the energy.

Table 2. The first four electron energy bands corresponding specific wave numbers k.

k (A^{o-1})	1^{st} energy band (eV)	2^{nd} energy band (eV)	3^{rd} energy band (eV)	4^{th} energy band (eV)
0	28.449	150.610	262.570	602.441
0.314	28.635	149.486	264.329	598.009
0.628	29.185	146.384	269.365	586.375
0.942	30.063	141.864	277.063	570.403
1.257	31.221	136.579	286.704	552.446
1.571	32.578	131.111	297.569	534.047
1.885	34.021	125.932	308.935	516.304
2.199	35.411	121.436	319.973	500.218
2.513	36.584	117.946	329.595	486.957
2.827	37.373	115.730	336.386	477.982
3.141	37.653	114.978	338.873	474.799

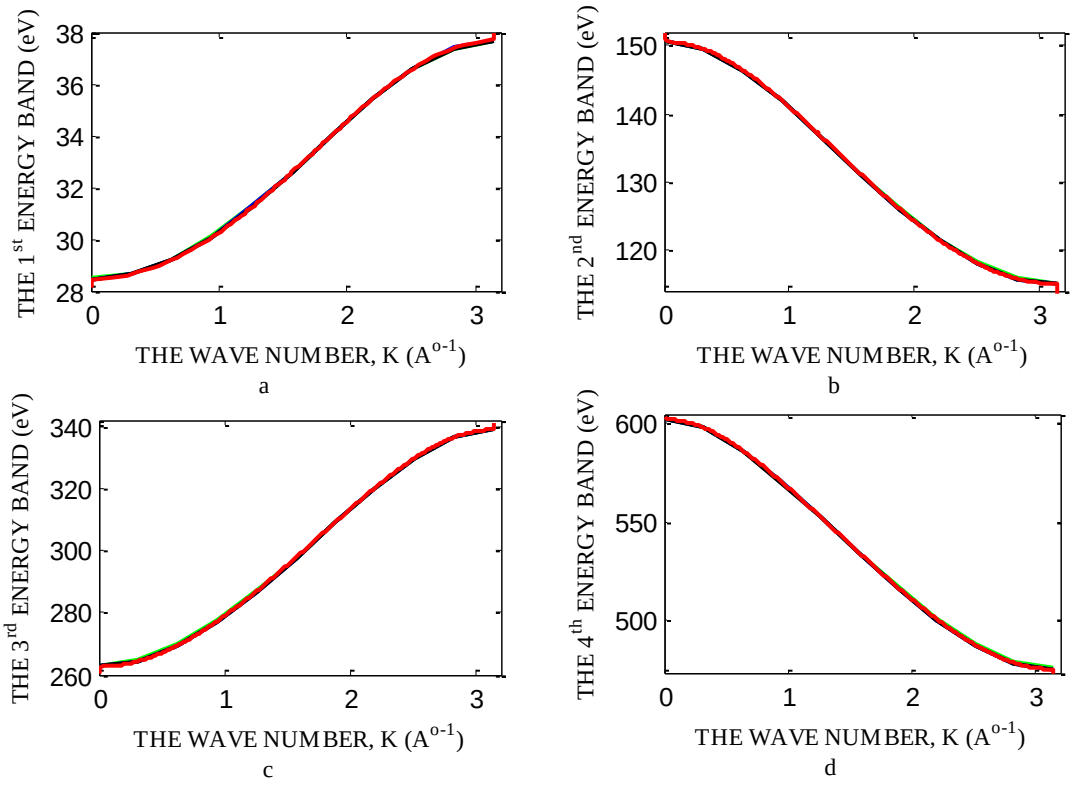

Figure 10. The first four electron energy bands in a one dimensional lattice with unit cell a = 1 A^o having a crntral delta function potential with V_0 = 100 eV calculated using different methods.

In the plane wave method, the Fourier coefficients of the delta function potential are given by

$$U_G = v_0, \tag{40}$$

where $v_0 = \frac{2m}{\hbar^2} V_0$.

The results in Fig. 10, are calculated by expanding the system to 100 plane waves which is numerically costing.

In the finite difference method the eigenvalus are calculated similarly to the previous square well potential, the wave function $\Psi(x_n)$ are calculated numerically by Eq. (28), while the wave function at the position of the delta-function is given by

$$\Psi_{\frac{N}{2}+1} = (v_0\Delta + 2)\Psi_{\frac{N}{2}} - \Psi_{\frac{N}{2}-1}. \tag{41}$$

The mesh size used in these results is $\Delta = 0.00001$

In the analytical solution the eigenvalues calculated by using Eq. (35), where the transmission coefficient of the delta function potential is given by

$$t = \frac{iK}{iK - \frac{v_0}{2}}, \tag{42}$$

and the reflection coefficient is given by [6]

$$r = \frac{\frac{v_0}{2}}{iK - \frac{v_0}{2}}. \tag{43}$$

Conclusion

In this paper, we have employed the transmission line method to calculate the electron energy bands in one dimensional lattice by applying a resonance condition of the impedance based on Bloch's theorem, this resonance condition involves an integral calculation as in Eq. (20). In Fig. 2 and Fig. 7 we have shown the impedance function as a function of distance for electron energy eigenvalues included in a high energy band for both the square well potential and the delta-function potential respectively, to explain how we modified Simpson Rule using Laurant Approximation to perform the integral involved in the resonance condition numerically. In Fig. 3 and Fig. 8, we demonstrate the resonance condition against the energy for the square well potential and the delta-function potential respectively in order to explain how we can get the electron energy bands by applying this condition. The resulting energy bands for the square well potential and the delta-function potential have been shown in Fig. 4 and Fig. 9, respectively, as a result, the width of the forbidden gabs become progressively narrower. We have presented a detailed account of the energy bands calculated numerically using different method and the energy bands calculated analytically to check our results against results from different methods. This comparison is illustrated in Fig. 5 and Fig. 10, for the square well potential and the delta-function potential respectively. The results of the transmission line method fit well with other numerical techniques and has the advantage of less expensive computations compared to the finite difference method and plane wave expansion.

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