

THEORETICAL ANALYSIS OF NANOMATERIALS USING MATLAB AS A TOOL

D. T. Dongare

S.S.S.K.R. Innani Mahavidyalaya, Karanja Lad Dist. Washim (M.S), India

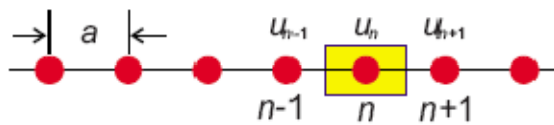
ABSTRACT

In this study, It has been tried to explain the dispersion relation (Energy versus k) and observe the wave functions for electron in nanomaterials using MATLAB as a tool. We have tried to predict the properties of mono atomic crystal without actually performing the experiments but using MATLAB as a tool to simulate its structure and electron wave function. A specific value of weight function has been assigned to each found in the system and unit cell is identified. Each atom in the unit cell is represented in the form of a matrix with adjacent weight functions taken into account. The wave functions and eigen values for the matrix were found out in MATLAB

Key words : MATLAB, eigen value, wavefunctions.

Introduction

1-D CHAIN OF ATOMS



We consider 1-D chain of atoms such that the wave function at 'n'th position is given by u_n and 'W' is the weight function indicating the extent of overlap (sharing of electron) between two neighbor atoms. Higher value of 'W' indicates higher sharing or overlap.

$$i\hbar \frac{\partial \Psi(r,t)}{\partial t} = H\Psi(r,t)$$

$$\Psi(r,t) = u(r,t)$$

$u(r,t)$ represents electronic wave function in a unit cell consisting of 1-atom.

$$i\hbar \frac{\partial \Psi(t)}{\partial t} = H\Psi(t)$$

$$(H - E)\Psi = 0$$

$P_n = |u_n|^2$ (Probability of finding electron at site 'n')

$$i\hbar \frac{d u_n}{dt} = -W(u_{n-1} + u_{n+1})$$

$$i \frac{d u_n}{dt} = H u_n = -(u_{n-1} + u_{n+1}) \dots \dots \dots (1)$$

$$E u_n = H u_n = -(u_{n-1} + u_{n+1}) \dots \dots \dots (2)$$

Then we consider 'T' to be a translation operator such that –

$$u_{n+1} = T u_n$$

And similarly,

$$u_n = T u_{n-1}$$

Thus,

$$u_{n-1} = T^{-1} u_n$$

Putting above values in equation (2), we get,

$$H u_n = -(T + T^{-1}) u_n$$

$$H = -(T + T^{-1}) \dots \dots \dots (3)$$

Thus from equation (3) we can say that Hamiltonian ‘H’ is a function of translation operator ‘T’ and thus,

$$[T, H] = 0$$

We know that ‘commuting operators can be characterized by same eigen functions’ and thus,

$$Tu_n = \lambda u_n$$

Replacing infinite lattice by periodic chain and using Bloch’s theorem, such that- $0 \leq n \leq N$

$u_N = T^N u_0 = \lambda^N u_0 = u_0$ (Operating translation operator on 0^{th} state N times will result in the same state)

$$\lambda^N = 1$$

$$\lambda = e^{\frac{i2\pi n}{N}}, n = 0, 1, 2, 3, \dots, (N-1).$$

$$\lambda_k = e^{\frac{i2\pi k}{N}} = e^{ik}$$

Where, $= \frac{2\pi m}{N}$, $m = 0, \pm 1, \pm 2, \dots$ (‘k’ is a wave vector (quasi-momentum of an electron))

$$\Delta k = \frac{2\pi}{N}$$

$$u_n = e^{ikn} u_0$$

Normalization gives us,

$$u_n = e^{ikn}$$

With the translation operator being :

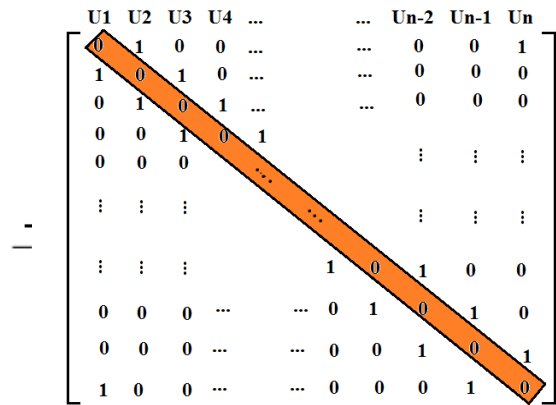
$$T = e^{ik} \dots \dots \dots (4)$$

Putting value from equation (4) to equation (2), we get,

$$E = H = -(e^{ik} + e^{-ik}) = -2 \cos k \dots \dots \dots (5)$$

Long wavelength approximation tells us the behaviour of the ‘E’ vs ‘k’ curve at excitations whose characteristic wavelength is much larger than lattice constant. i.e. k (which is nothing but $\frac{2\pi}{\lambda}$ is very small).then :

$$E = -2 \cos k = -2 \left(1 - \frac{k^2}{2}\right) = -2 + k^2.$$



If we have continuous distribution in place of discrete atoms (wave-like behavior) then we will replace ‘x’ in place of ‘n’ for above equations and equation (1) will be :

$$i \frac{d u(x)}{dt} = H u(x) = -(u(x-1) + u(x+1))$$

Taylor series expansion upto first few terms will give,

$$i \frac{d u(x)}{dt} = - \left[u(x) - \frac{\partial u(x)}{\partial x} + \frac{\partial^2 u(x)}{\partial x^2} + u(x) + \frac{\partial u(x)}{\partial x} + \frac{\partial^2 u(x)}{\partial x^2} \right] = - \left[2 + \frac{\partial^2}{\partial x^2} \right] u(x)$$

MATLAB Method

```

Clear
N=100
%specifying matrix dimensions by 'N'
u = zeros( N , N ) ;
u ( 1 , 2 ) = 1 ;
u ( 1 , N ) = 1 ;
for i = 2 : N - 1
    u ( i , i - 1 ) = 1 ;
    u ( i , i + 1 ) = 1 ;
end
% We made above matrix following the
relations among consecutive atoms
% Considering 1 atom in a unit cell such
that-
%  $i(\hbar/(2*\pi))(du(n)/dt) = -W(u(n-1)+u(n+1))$ 
[ Z , x ] = eig(u) ;
% Z denotes a matrix in which each column
represents a wave function and x is
% A diagonal matrix with diagonal elements
representing eigen values.
y(1:N+2,1:N)=0;
y(2:N+1,1:N)=Z;
% Above conditions employed to incorporate
the boundary conditions where
% Wave function should vanish, so first row
and last row of wave function
% Matrix Z is made '0'.
s = 1 : N + 2 ;
s = s / N + 2 ;
% For normalization we divided by (N+2)
s1 = 1 : N ;
% s1=s1/N;
p=1;
figure(1)
plot(s,y(:,p),'r')
% To plot 'p'th wave function (i.e.'p'th
column of matrix 'y')
figure(2)
for s1=1:100
plot(s1,x(s1,s1),'')
hold on;
end
% To plot energy eigen values
Z;
y;
x;

```

Figure1 : Energy eigen value vs. K

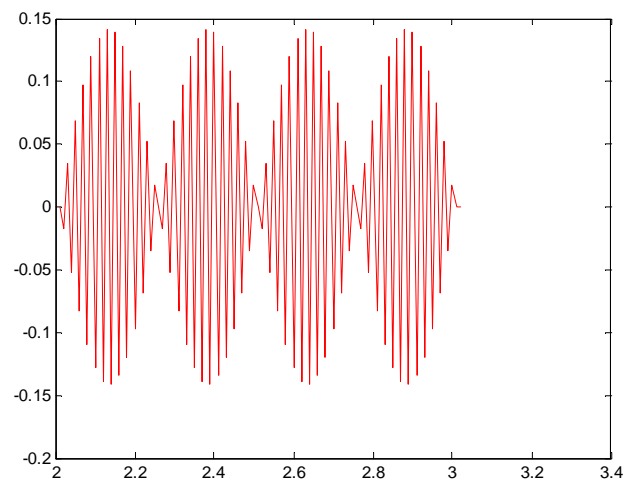
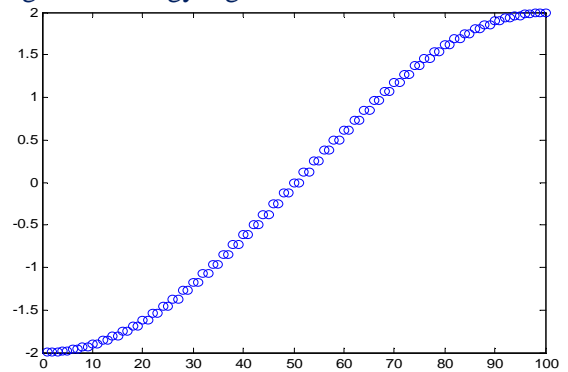


Figure2: result of program

Result and Discussion

The above examples clearly show that if we know the structure of a nanomaterial and the extent of overlap in its adjacent atoms, we can find out the dispersion relation for the lattice structure. The folding of the Brillouin zone and the restriction to passage of a range of wavelengths can easily be seen from the plots in MATLAB. This method will definitely prove useful to teach nanomaterials and to give clear idea of their properties in class rooms. This tool can be used to model any material if its structure and bonding is known.

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