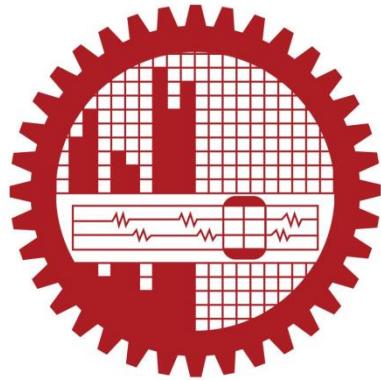


BANGLADESH UNIVERSITY OF ENGINEERING AND TECHNOLOGY



## ASSIGNMENT 2

Course No: EEE 6502

Course Title: Electronics of Solids

Course Teacher: Dr. Mahbub Alam

**Submitted by:**

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Semester: 1'st

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## Problem 1:

Objectives:

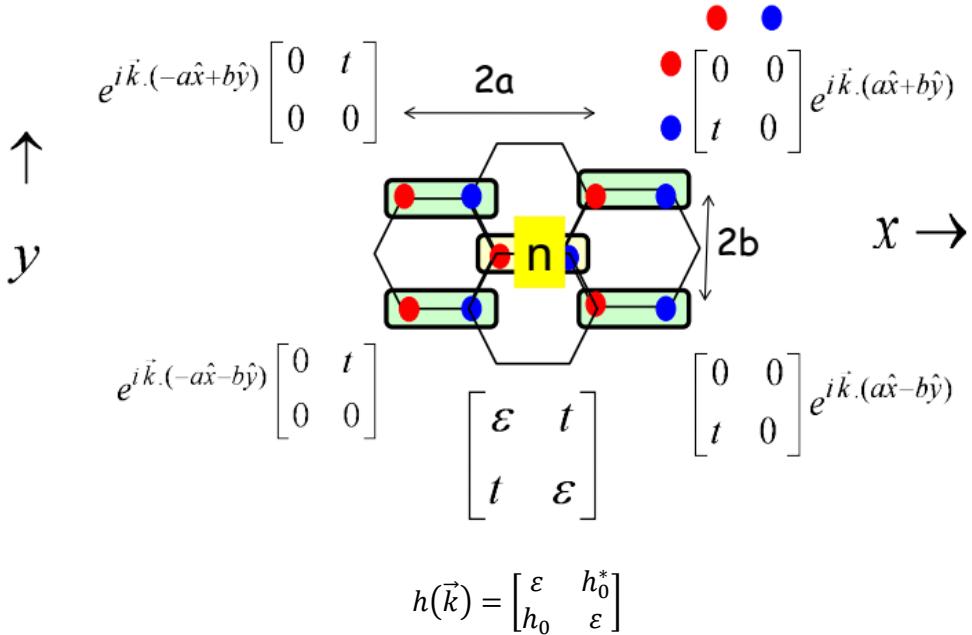
To draw the E-k diagram of bulk Graphene both analytically and numerically.

Procedure:

The energy levels can be determined from the eigenvalues of the matrix

$$[h(\vec{k})] = \sum_m [H_{nm}] e^{i\vec{k} \cdot (\vec{r}_m - \vec{r}_n)}$$

We determine  $h(\vec{k})$  as following



$$h(\vec{k}) = \begin{bmatrix} \epsilon & h_0^* \\ h_0 & \epsilon \end{bmatrix}$$

Numerical method:

Ignoring the constant potential energy:

$$h(\vec{k}) = \begin{bmatrix} 0 & h_0^* \\ h_0 & 0 \end{bmatrix}$$

Where,

$$h_0 = -t(1 + e^{ik_x a + ik_y b} + e^{ik_x a - ik_y b})$$

Analytical method:

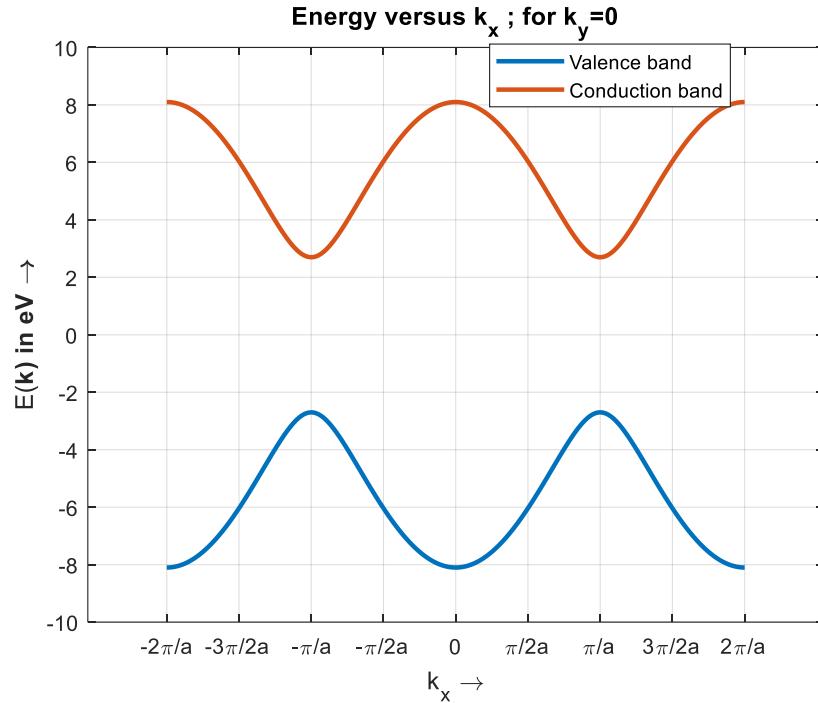
$$h_0 = -t(1 + 2e^{ik_x a} \cos k_y b)$$

$$E = \pm |h_0|$$

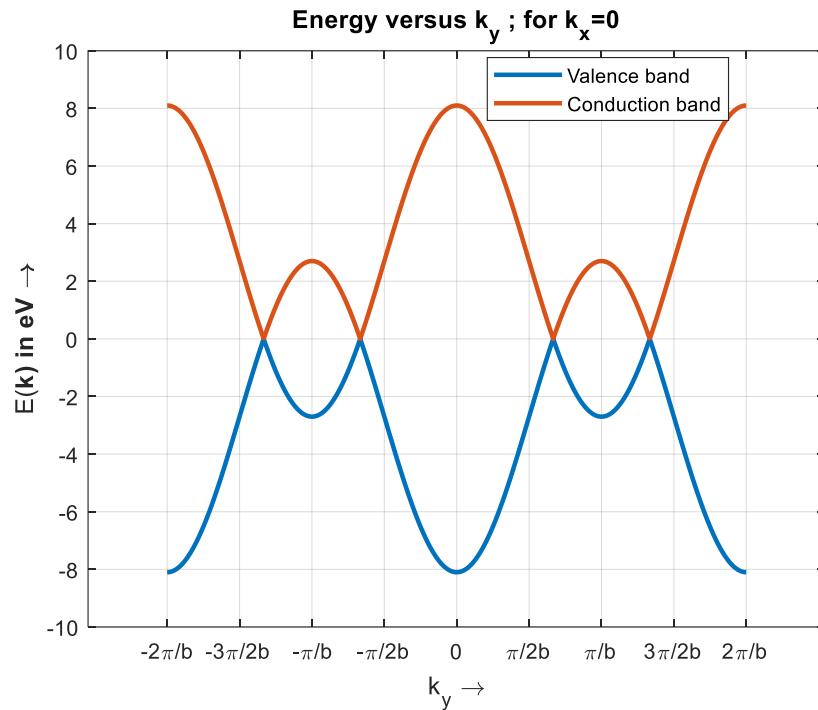
Results:

Analytical results:

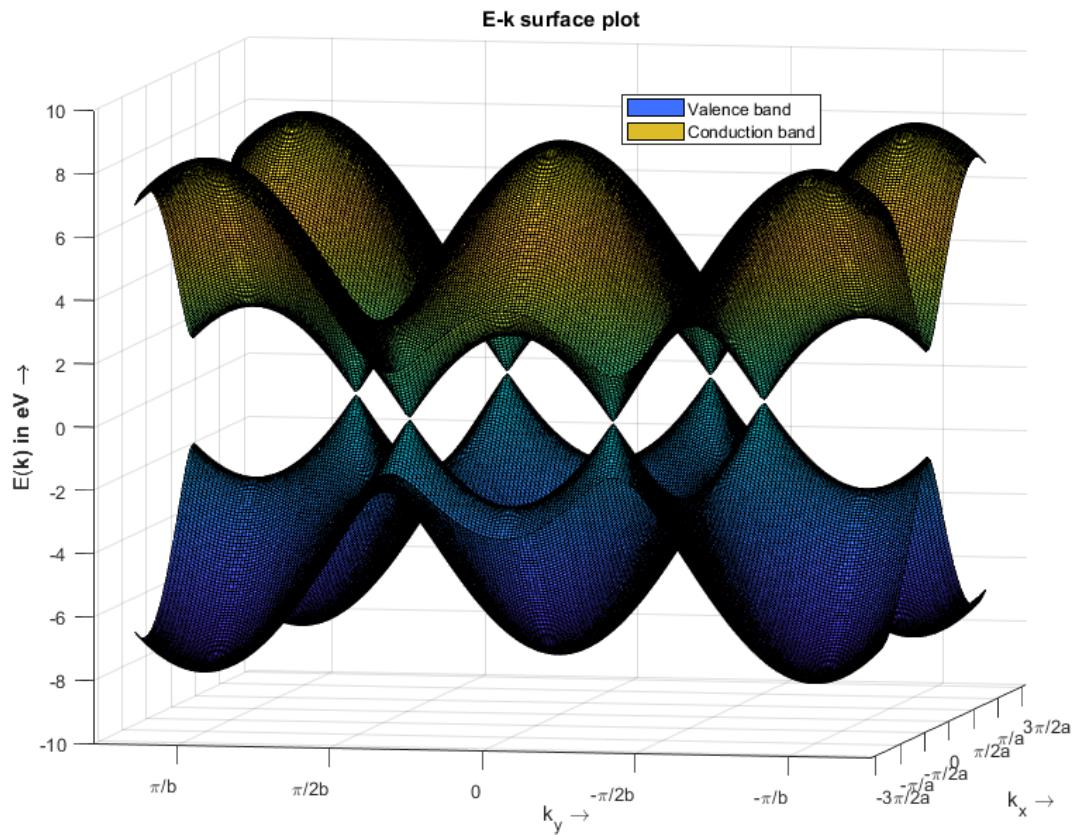
*Energy versus  $k_x$ ; for  $k_y = 0$*



*Energy versus  $k_y$ ; for  $k_x = 0$*

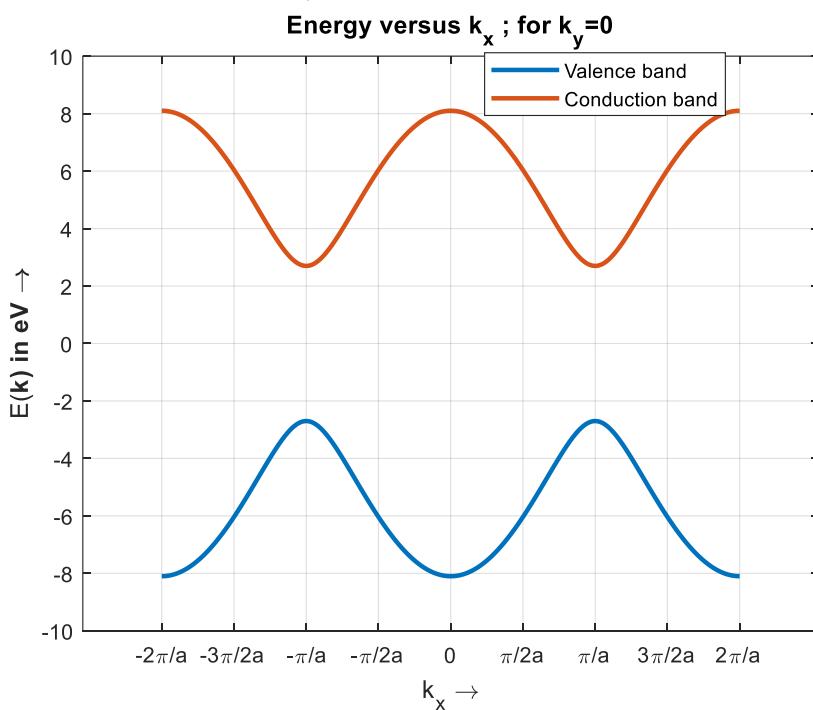


E-k surface plot:

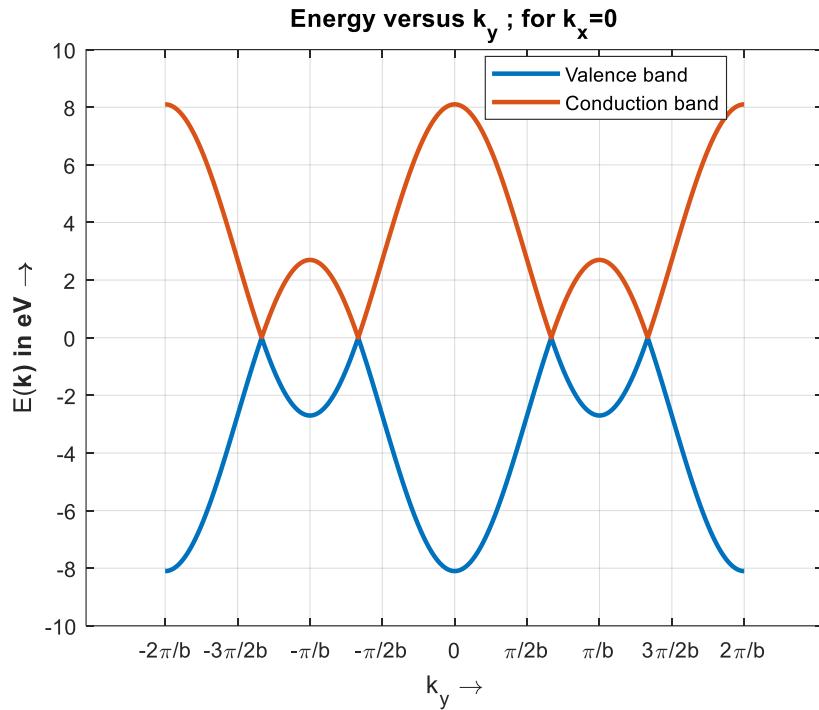


Numerical results:

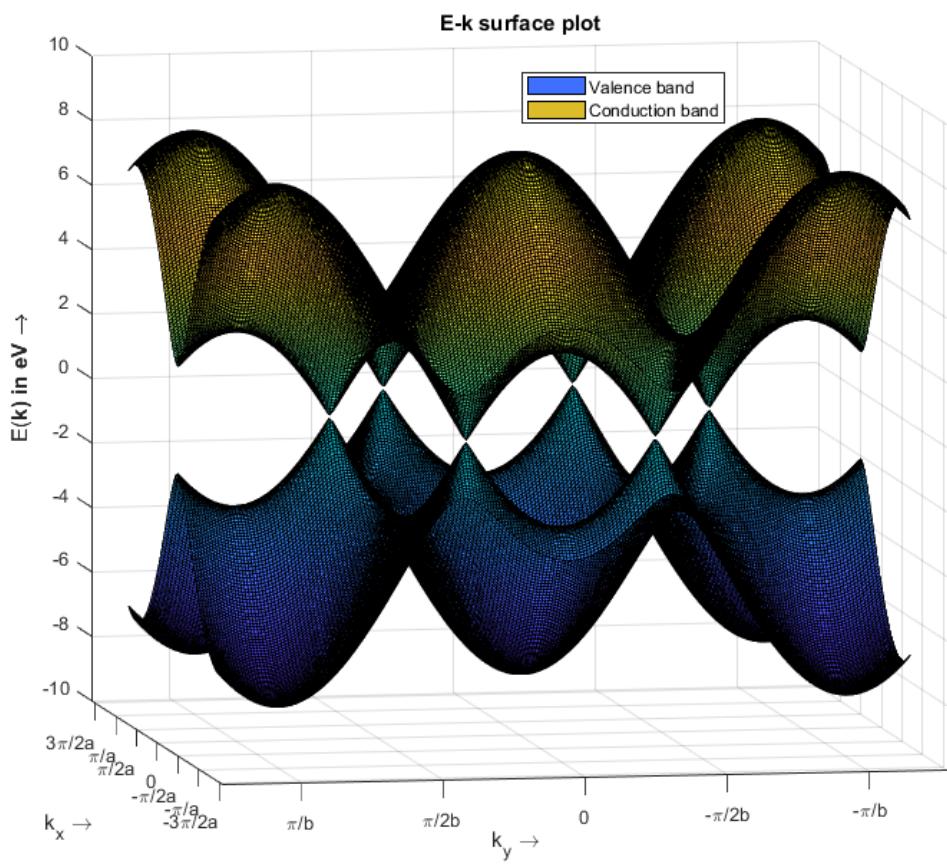
*Energy versus  $k_x$ ; for  $k_y = 0$*



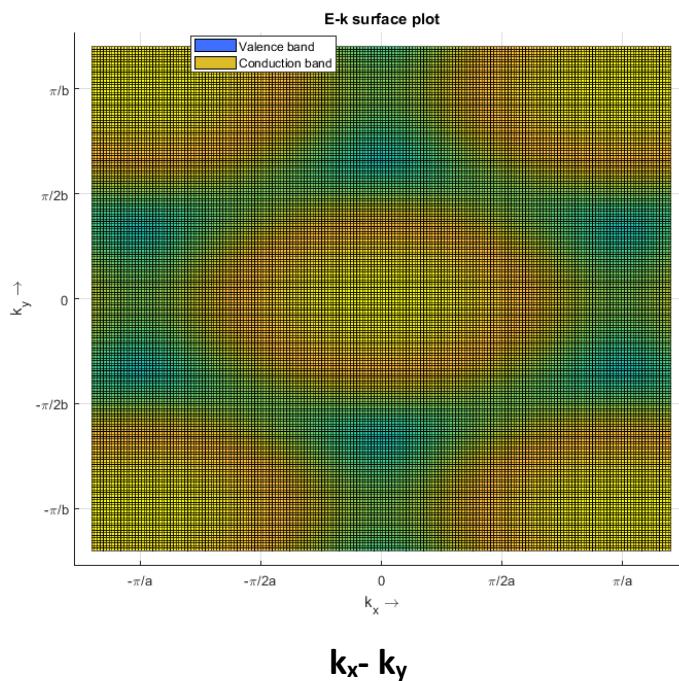
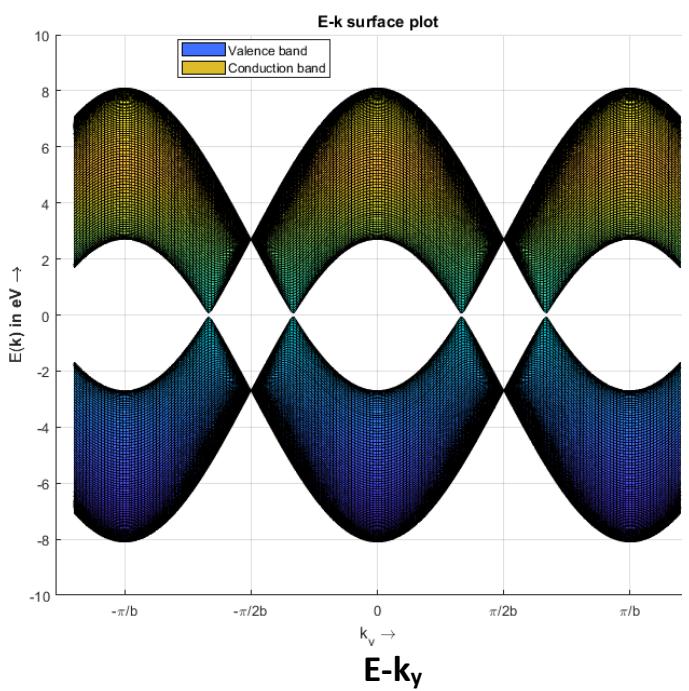
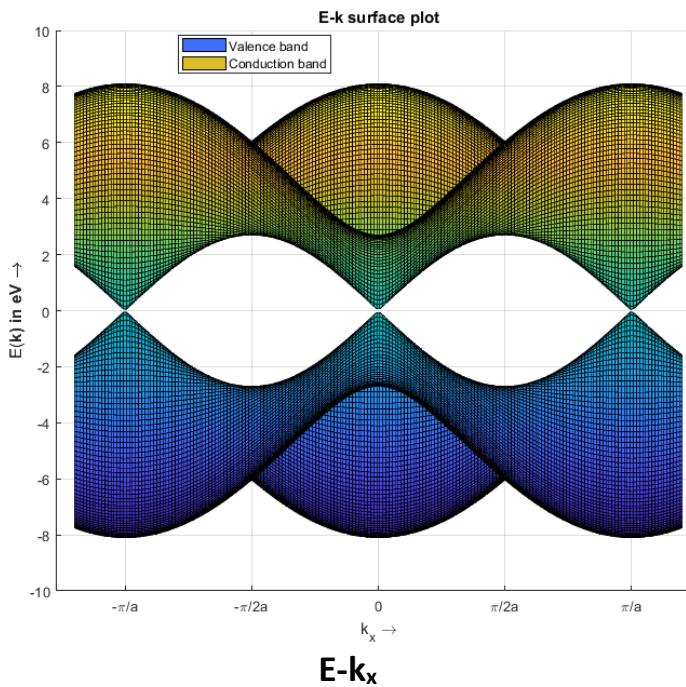
*Energy versus  $k_y$ ; for  $k_x = 0$*



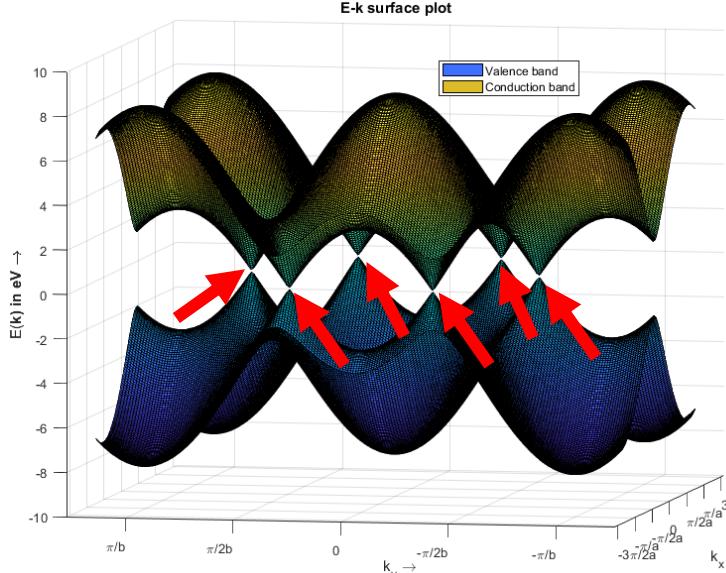
E-k surface plot:



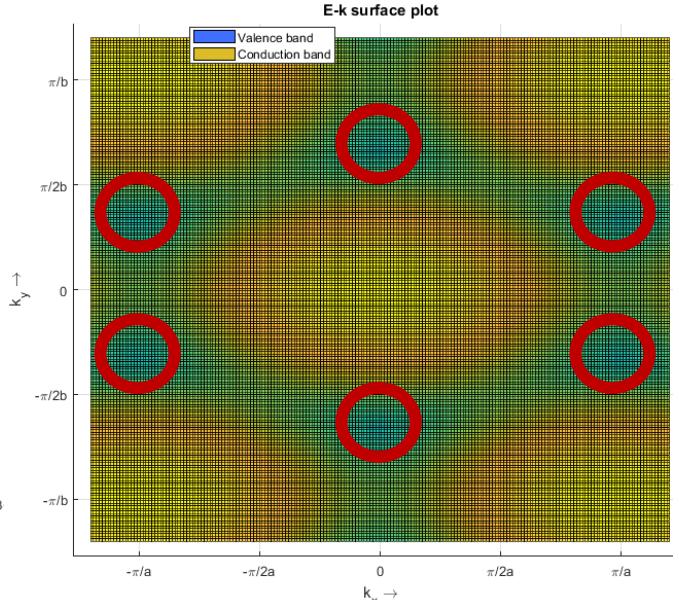
Surface plot from different viewpoints:



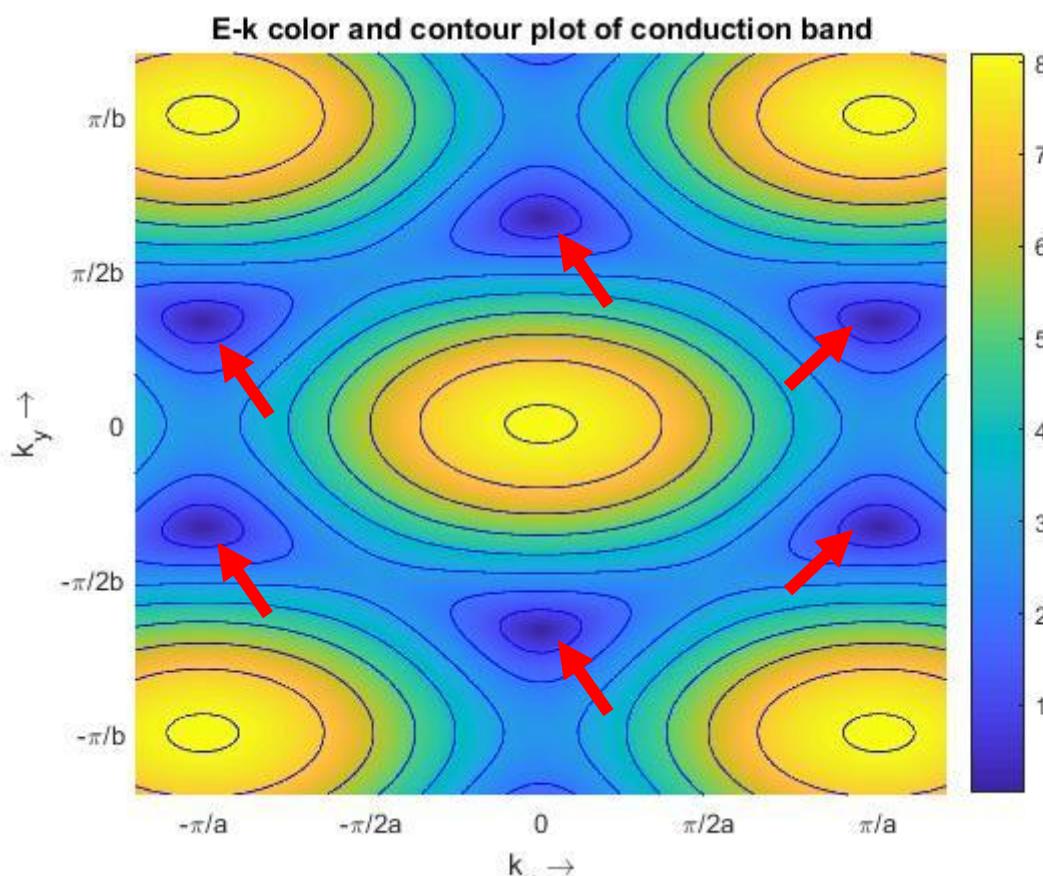
## High Symmetry Points: in different views



Isometric view of surface plot



Top view of surface plot



Contour plot of conduction band

## Discussions:

- Bulk Graphene has no bandgap, i.e. bandgap =0. The conduction and valence bands touch each other.
- The lack of a bandgap is the reason for the metallic nature of the bulk grapheme.
- There are six points of high symmetry in the band structure of bulk graphene at  $(k_x a, k_y b) = \left(0, \pm \frac{2\pi}{3}\right), \left(\pm\pi, \pm \frac{\pi}{3}\right)$  as observed from the surface and colour plots. The bandgap is zero at these points.
- The E-k relationship in the vicinity of the high symmetry points is almost linear. This results in the ‘nearly massless’ nature of electron in grapheme.
- Both analytical and numerical analysis give the same results.

## Problem 2:

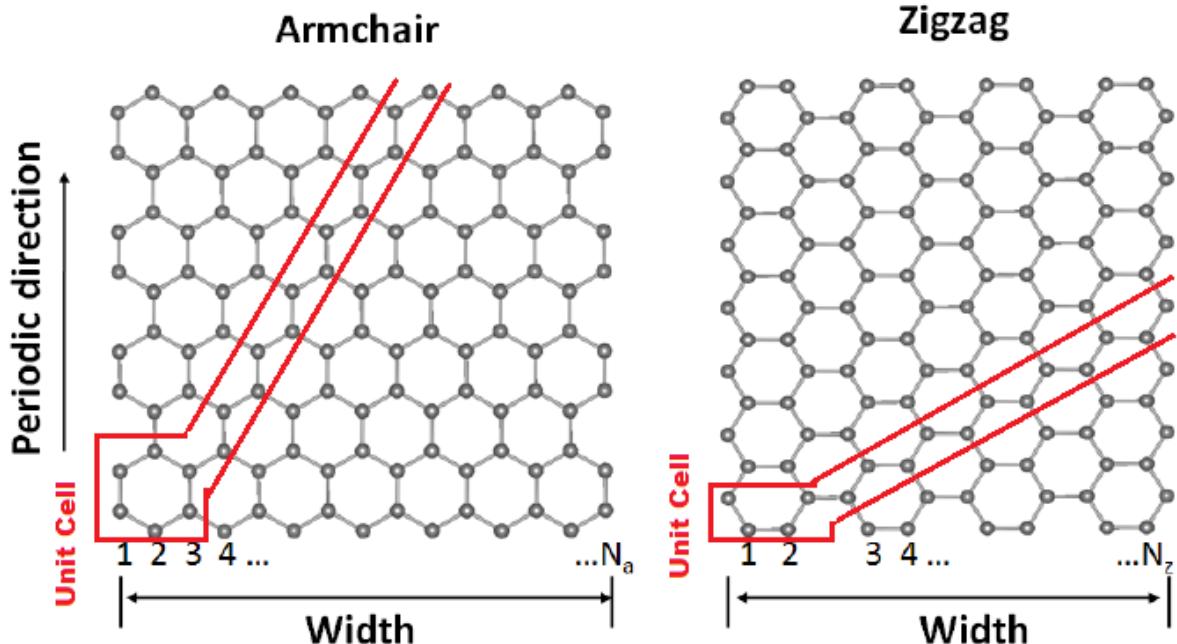
### Objectives:

To draw the band structures of armchair and zigzag Graphene nano-ribbons numerically.

### Procedure:

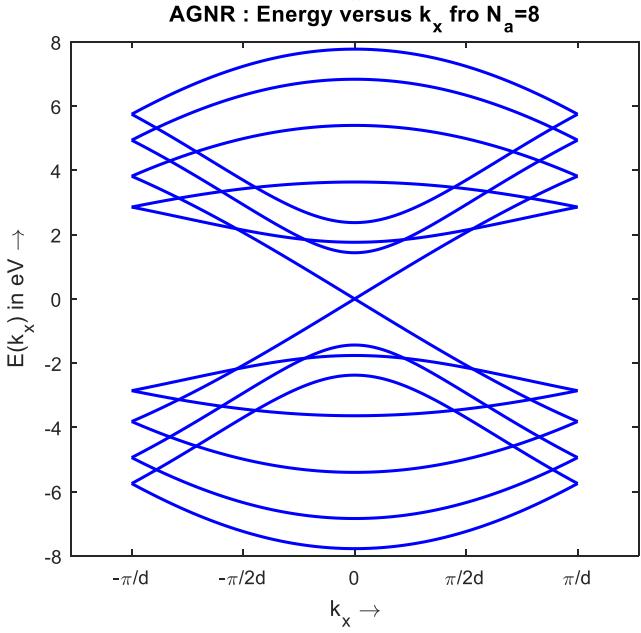
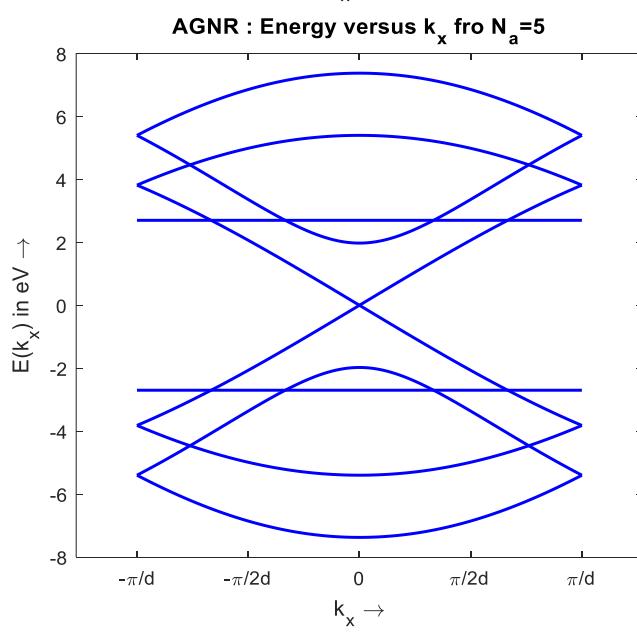
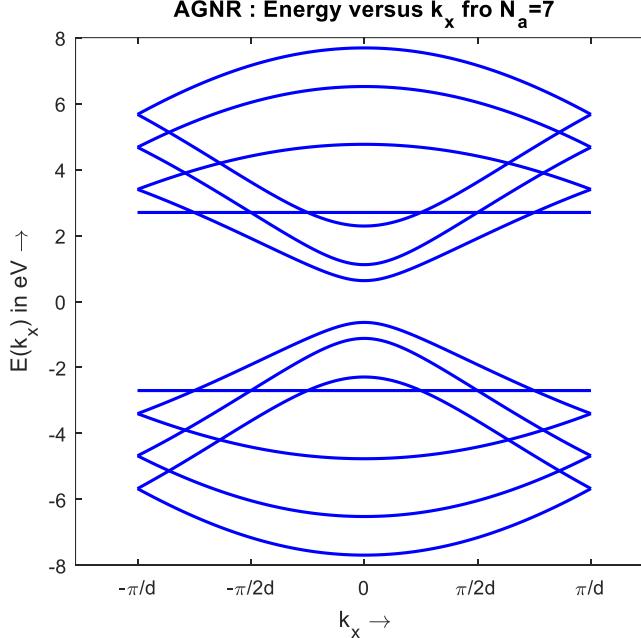
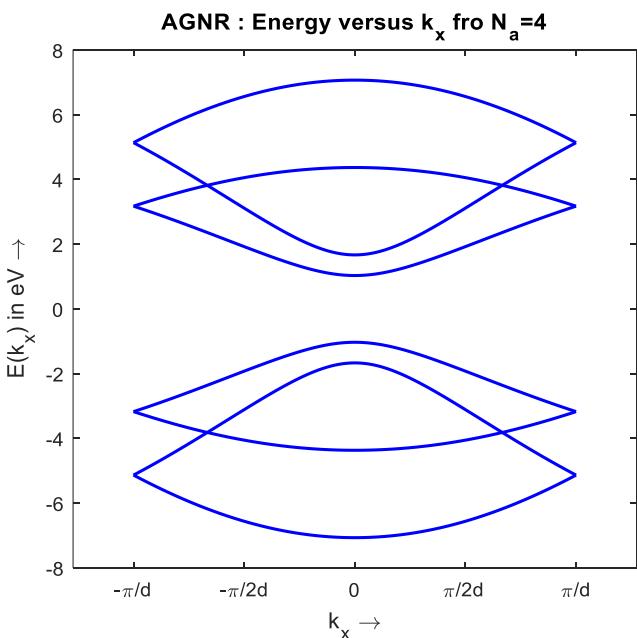
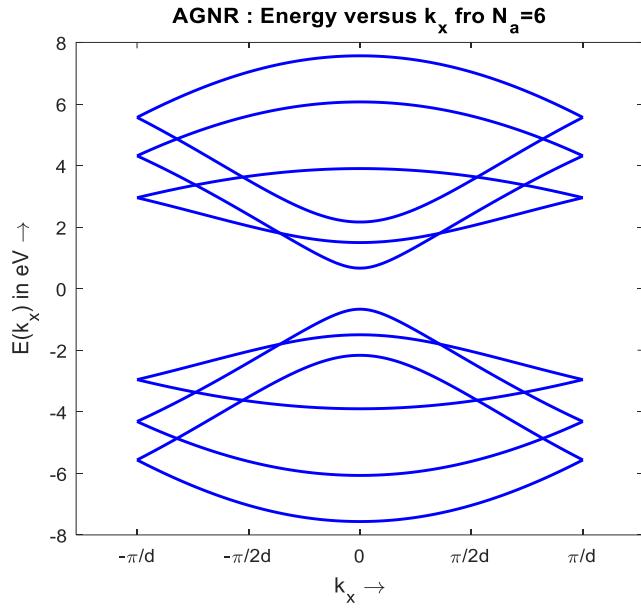
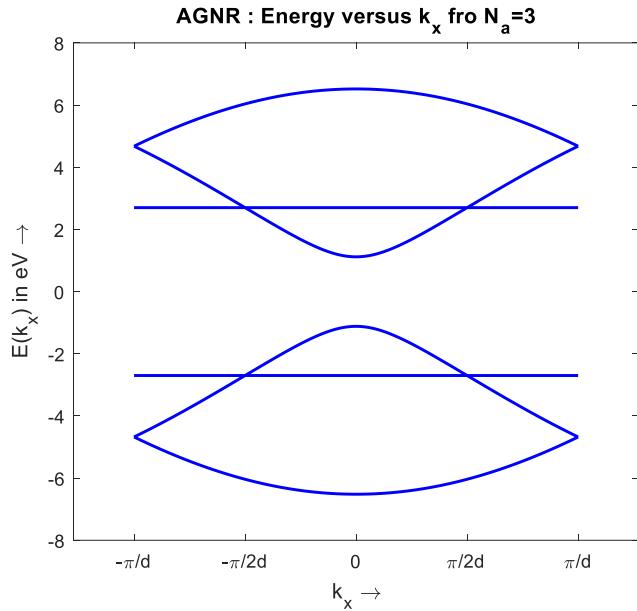
The energy levels can be determined from the eigenvalues of the matrix

$$[h(\vec{k})] = \sum_m [H_{nm}] e^{i\vec{k} \cdot (\vec{r}_m - \vec{r}_n)}$$

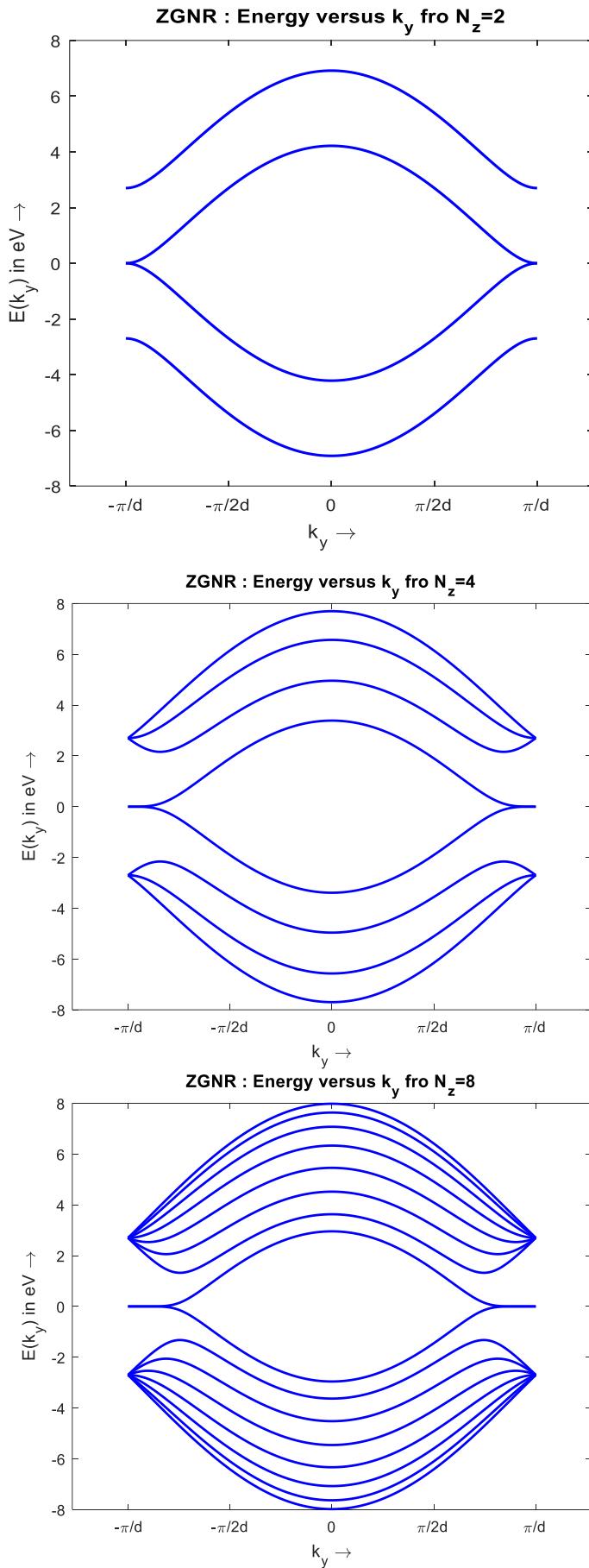


- First a proper unit cell is chosen for the ribbon given the particular width of the ribbon.
- Then we apply the nearest neighbor approximation to find  $h(\vec{k})$ .
- We perform eigenvalue analysis on  $h(\vec{k})$  for different values of  $k$ .
- Each eigenvalue corresponds to energy in a particular band for a given value of  $k$ .

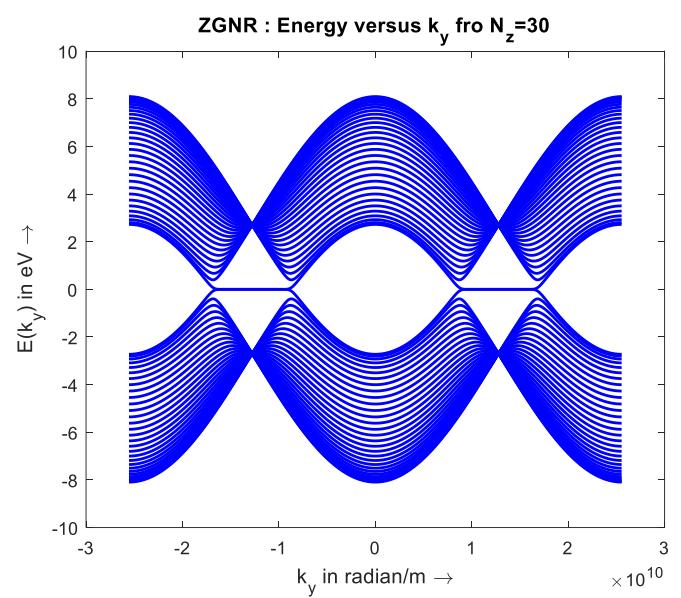
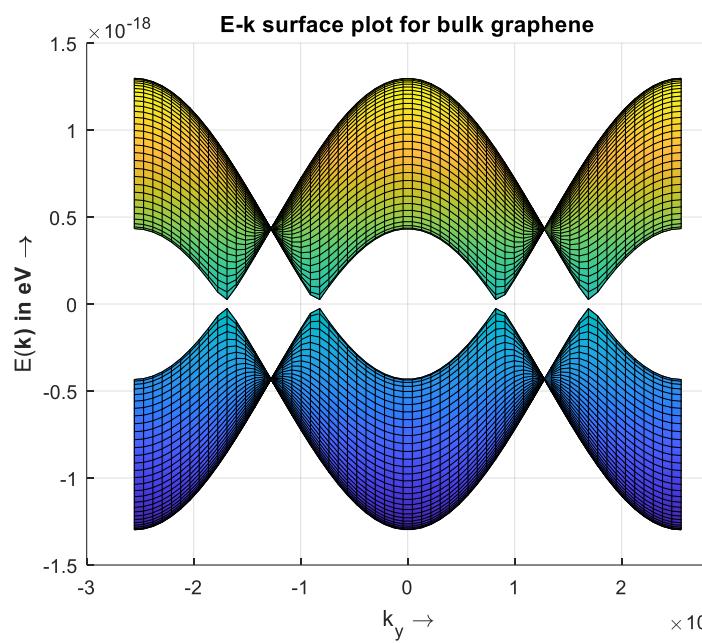
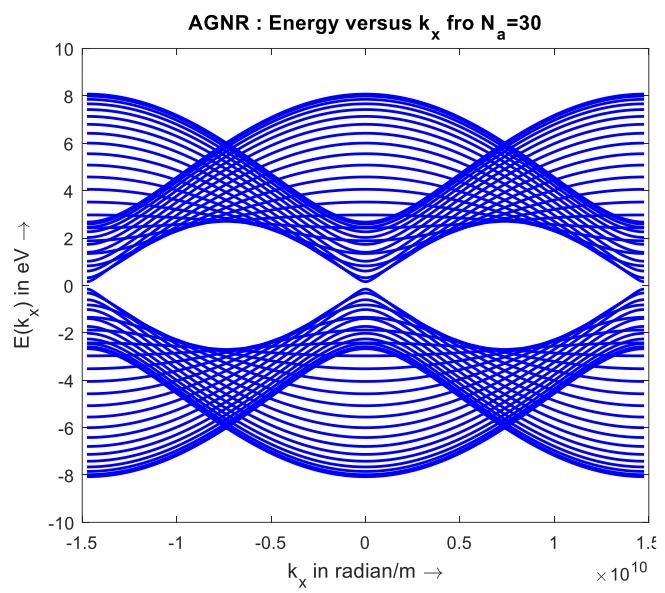
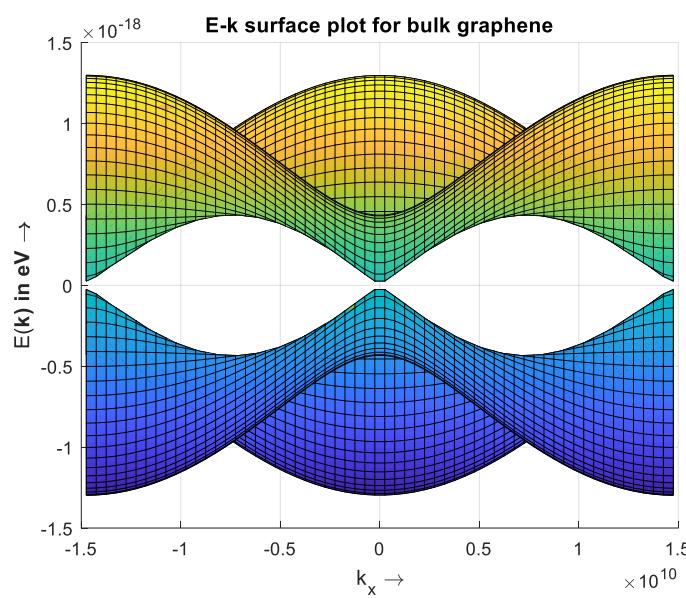
## Results: Armchair GNR:



## Results: Zigzag GNR:



## Comparison between bulk Graphene and wide GNR:



## Discussions:

- The simple tight binding model predicts that Zigzag GNR has no bandgap, regardless of its width (although more advanced models that consider spin, show that this is not true).
- Narrow Armchair GNR has a bandgap like semiconductors for particular values of  $N_a$ . So it can be used in electronics (for example: to make transistors).
- The bandgap of AGNR closes for  $N_a = 3l + 2; l \in \mathbb{Z}$ , and conduction and valence band touch for these particular widths. So, the GNR loses its semiconducting properties and becomes metallic.
- The bandgap of AGNR decreases with increasing width.
- The band structure of wide AGNR looks like that of bulk graphene sampled along the  $k_y$  axis.
- The band structure of wide ZGNR looks like that of bulk graphene sampled along the  $k_x$  axis.

## Appendix: Matlab codes for generating plots:

### Problem 1: Analytical:

```
clc; clear all; close all

h_cut = 1.055e-34;
eV = 1.602e-19;
Armst=1e-10;

ep0_eV=0;
t_eV=2.7;
a0_A0=1.42;

ep0=ep0_eV*eV;
t=t_eV*eV;
a0=a0_A0*Armst;

a=3*a0/2;
b=sqrt(3)*a0/2;
a1=[a,b];
a2=[a,-b];

res=1e3;
rang=2*pi/a;
kx=linspace(-rang,rang,res);
ky=zeros(1,res);
kv=[kx; ky];
Ev=zeros(size(kv));

for i=1:length(kv)
    k=kv(:,i);
    h0=-t*(1+2*exp(1i*k(1)*a)*cos(k(2)*b));
    h0a=abs(h0);
    Ev(:,i)=[-h0a;h0a];
end

figure
plot(kx*a,Ev(1,:)/eV, 'LineWidth', 2)
grid on;hold on
plot(kx*a,Ev(2,:)/eV, 'LineWidth', 2)
xlabel('k_x \rightarrow');ylabel('E(\bf{k}) in eV \rightarrow')
xticks([-2*pi -3*pi/2 -pi -pi/2 0 pi/2 pi 3*pi/2 2*pi]);
xticklabels({'-2\pi/a', '-3\pi/2a', '-\pi/a', '-\pi/2a', '0', '\pi/2a', '\pi/a', '3\pi/2a', '2\pi/a'})
title('Energy versus k_x ; for k_y=0')
legend('Valence band', 'Conduction band');

rang=2*pi/b;
kx=zeros(1,res);
ky=linspace(-rang,rang,res);
kv=[kx; ky];
Ev=zeros(size(kv));

for i=1:res
    k=kv(:,i);
    h0=-t*(1+2*exp(1i*k(1)*a)*cos(k(2)*b));
    h0a=abs(h0);
    Ev(:,i)=[-h0a;h0a];
end
```

```

figure
plot(ky*b,Ev(1,:)/eV, 'LineWidth', 2)
grid on;hold on
plot(ky*b,Ev(2,:)/eV, 'LineWidth', 2)
xlabel('k_y \rightarrow');ylabel('E(\bf{k}) in eV \rightarrow')
xticks([-2*pi -3*pi/2 -pi -pi/2 0 pi/2 pi 3*pi/2 2*pi]);
xticklabels({'-2\pi/b', '-3\pi/2b', '-\pi/b', '-\pi/2b', '0', '\pi/2b', '\pi/b', '3\pi/2b', '2\pi/b'})
title('Energy versus k_y ; for k_x=0')
legend('Valence band', 'Conduction band');

res=2e2;
kx=linspace(-6/5*pi/a,6/5*pi/a,res);
ky=linspace(-6/5*pi/b,6/5*pi/b,res);
[Kx,Ky]=meshgrid(kx,ky);
kv=[Kx(:).';Ky(:).'];
Ev=zeros(size(kv));

for i=1:length(kv)
    k=kv(:,i);
    h0=-t*(1+2*exp(li*k(1)*a)*cos(k(2)*b));
    h0a=abs(h0);
    Ev(:,i)=[-h0a;h0a];
end

E1=reshape(Ev(1,:),res,res);
E2=reshape(Ev(2,:),res,res);

figure
h1=surf(Kx*a,Ky*b,E1/eV);
hold on
h2=surf(Kx*a,Ky*b,E2/eV);
shading interp
set(h1,'edgecolor','k');set(h2,'edgecolor','k')
xlabel('k_x \rightarrow');ylabel('k_y \rightarrow');zlabel('E(\bf{k}) in eV \rightarrow')
xticks([-2*pi -3*pi/2 -pi -pi/2 0 pi/2 pi 3*pi/2 2*pi]);
yticks([-2*pi -3*pi/2 -pi -pi/2 0 pi/2 pi 3*pi/2 2*pi]);
xticklabels({'-2\pi/a', '-3\pi/2a', '-\pi/a', '-\pi/2a', '0', '\pi/2a', '\pi/a', '3\pi/2a', '2\pi/a'})
yticklabels({'-2\pi/b', '-3\pi/2b', '-\pi/b', '-\pi/2b', '0', '\pi/2b', '\pi/b', '3\pi/2b', '2\pi/b'})
title('E-k surface plot')
legend('Valence band', 'Conduction band');

figure
pcolor(Kx*a,Ky*b,E2/eV);
shading('interp');
hold on
contour(Kx*a,Ky*b,E2/eV, 'LineColor', 'b');
colorbar
xlabel('k_x \rightarrow');ylabel('k_y \rightarrow');zlabel('E(\bf{k}) in eV \rightarrow')
xticks([-2*pi -3*pi/2 -pi -pi/2 0 pi/2 pi 3*pi/2 2*pi]);
yticks([-2*pi -3*pi/2 -pi -pi/2 0 pi/2 pi 3*pi/2 2*pi]);
xticklabels({'-2\pi/a', '-3\pi/2a', '-\pi/a', '-\pi/2a', '0', '\pi/2a', '\pi/a', '3\pi/2a', '2\pi/a'})
yticklabels({'-2\pi/b', '-3\pi/2b', '-\pi/b', '-\pi/2b', '0', '\pi/2b', '\pi/b', '3\pi/2b', '2\pi/b'})
title('E-k color and contour plot of conduction band')

```

## Problem 1: Numerical:

```
clc; clear all; close all

h_cut = 1.055e-34;
eV = 1.602e-19;
Armst=1e-10;

ep0_eV=0;
t_eV=2.7;
a0_A0=1.42;

ep0=ep0_eV*eV;
t=t_eV*eV;
a0=a0_A0*Armst;

a=3*a0/2;
b=sqrt(3)*a0/2;
a1=[a;b];
a2=[a;-b];

res=1e3;
rang=2*pi/a;
kx=linspace(-rang,rang,res);
ky=zeros(1,res);
kv=[kx; ky];
Ev=zeros(size(kv));

for i=1:length(kv)
    k=kv(:,i);
    h0=-t*(1+exp(1i*a1'*k)+exp(1i*a2'*k));
    hk=[ep0, conj(h0); h0, ep0];
    Ev(:,i)=eig(hk);
end

figure
plot(kx*a,Ev(1,:)/eV, 'LineWidth', 2)
grid on;hold on
plot(kx*a,Ev(2,:)/eV, 'LineWidth', 2)
xlabel('k_x \rightarrow');ylabel('E(\bf{k}) in eV \rightarrow')
xticks([-2*pi -3*pi/2 -pi -pi/2 0 pi/2 pi 3*pi/2 2*pi]);
xticklabels({'-2\pi/a', '-3\pi/2a', '-\pi/a', '-\pi/2a', '0', '\pi/2a', '\pi/a', '3\pi/2a', '2\pi/a'})
title('Energy versus k_x ; for k_y=0')
legend('Valence band','Conduction band');

rang=2*pi/b;
kx=zeros(1,res);
ky=linspace(-rang,rang,res);
kv=[kx; ky];
Ev=zeros(size(kv));

for i=1:res
    k=kv(:,i);
    h0=-t*(1+exp(1i*a1'*k)+exp(1i*a2'*k));
    hk=[ep0, conj(h0); h0, ep0];
    Ev(:,i)=eig(hk);
end

figure
```

```

plot(ky*b,Ev(1,:)/eV, 'LineWidth', 2)
grid on;hold on
plot(ky*b,Ev(2,:)/eV, 'LineWidth', 2)
xlabel('k_y \rightarrow');ylabel('E(\bf{k}) in eV \rightarrow')
xticks([-2*pi -3*pi/2 -pi -pi/2 0 pi/2 pi 3*pi/2 2*pi]);
xticklabels({'-2\pi/b', '-3\pi/2b', '-\pi/b', '-\pi/2b', '0', '\pi/2b', '\pi/b', '3\pi/2b', '2\pi/b'})
title('Energy versus k_y ; for k_x=0')
legend('Valence band', 'Conduction band');

res=2e2;
kx=linspace(-6/5*pi/a,6/5*pi/a,res);
ky=linspace(-6/5*pi/b,6/5*pi/b,res);
[Kx,Ky]=meshgrid(kx,ky);
kv=[Kx(:).';Ky(:).'];
Ev=zeros(size(kv));

for i=1:length(kv)
    k=kv(:,i);
    h0=-t*(1+exp(1i*a1'*k)+exp(1i*a2'*k));
    hk=[ep0, conj(h0); h0, ep0];
    Ev(:,i)=eig(hk);
end

E1=reshape(Ev(1,:),res,res);
E2=reshape(Ev(2,:),res,res);

figure
h1=surf(Kx*a,Ky*b,E1/eV);
hold on
h2=surf(Kx*a,Ky*b,E2/eV);
shading interp
set(h1,'edgecolor','k');set(h2,'edgecolor','k')
xlabel('k_x \rightarrow');ylabel('k_y \rightarrow');zlabel('E(\bf{k}) in eV \rightarrow')
xticks([-2*pi -3*pi/2 -pi -pi/2 0 pi/2 pi 3*pi/2 2*pi]);
yticks([-2*pi -3*pi/2 -pi -pi/2 0 pi/2 pi 3*pi/2 2*pi]);
xticklabels({'-2\pi/a', '-3\pi/2a', '-\pi/a', '-\pi/2a', '0', '\pi/2a', '\pi/a', '3\pi/2a', '2\pi/a'})
yticklabels({'-2\pi/b', '-3\pi/2b', '-\pi/b', '-\pi/2b', '0', '\pi/2b', '\pi/b', '3\pi/2b', '2\pi/b'})
title('E-k surface plot')
legend('Valence band', 'Conduction band');

figure
pcolor(Kx*a,Ky*b,E2/eV);
shading('interp');
hold on
contour(Kx*a,Ky*b,E2/eV, 'LineColor', 'b');
colorbar
xlabel('k_x \rightarrow');ylabel('k_y \rightarrow');zlabel('E(\bf{k}) in eV \rightarrow')
xticks([-2*pi -3*pi/2 -pi -pi/2 0 pi/2 pi 3*pi/2 2*pi]);
yticks([-2*pi -3*pi/2 -pi -pi/2 0 pi/2 pi 3*pi/2 2*pi]);
xticklabels({'-2\pi/a', '-3\pi/2a', '-\pi/a', '-\pi/2a', '0', '\pi/2a', '\pi/a', '3\pi/2a', '2\pi/a'})
yticklabels({'-2\pi/b', '-3\pi/2b', '-\pi/b', '-\pi/2b', '0', '\pi/2b', '\pi/b', '3\pi/2b', '2\pi/b'})
title('E-k color and contour plot of conduction band')

```

## Problem 2: Armchair GNR

```
clc; clear all; close all

h_cut = 1.055e-34;
eV = 1.602e-19;
Armst=1e-10;

t_eV=2.7;
a0_A0=1.42;

t=t_eV*eV;
a0=a0_A0*Armst;
a=3*a0/2;
d12=2*a;

na=30;
n=na-2;
d=6+(n-1)*2;
sn=[1:6; [2:6,1]];
tn=[5;2];
for m=2:n
    nm=(7+(m-2)*2):(8+(m-2)*2);
    if m==2
        c1=4;
    else
        c1=nm(1)-1;
    end
    nc=[nm(1:end-1),c1;nm(2:end),nm(1)];
    sn=[sn,nc];
    if m==2
        tn=[tn,[nm(end);3]];
    else
        tn=[tn,[nm(end);nm(1)-2]];
    end
end

res=1e3;
kv=linspace(-pi/d12,pi/d12,res);
Ev=zeros(d,length(kv));

for m=1:length(kv)
    k=kv(m);
    i=[sn(1,:),sn(2,:),tn(1,:),tn(2,:)];
    j=[sn(2,:),sn(1,:),tn(2,:),tn(1,:)];
    v=[repmat(-t, 1,2*size(sn,2)),repmat(-t*exp(1i*k*d12),
    1,size(tn,2)),repmat(-t*exp(-1i*k*d12),1, size(tn,2))];

    hk=sparse(i,j,v,d,d);
    egv=eig(full(hk));
    Ev(:,m)=egv;
end

figure
plot(kv*d12,Ev/eV, 'b', 'LineWidth',1.5)
xlabel('k_x \rightarrow'); ylabel('E(k_x) in eV \rightarrow')
xticks([-pi -pi/2 0 pi/2 pi]);
xticklabels({'-\pi/d', '-\pi/2d', '0', '\pi/2d', '\pi/d'});
title(['AGNR : Energy versus k_x fro N_a=',num2str(na)])
```

## Problem 2: Zigzag GNR

```
clc; clear all; close all

h_cut = 1.055e-34;
eV = 1.602e-19;
Armst=1e-10;

t_eV=2.7;
a0_A0=1.42;

t=t_eV*eV;
a0=a0_A0*Armst;
b=sqrt(3)*a0/2;
d12=2*b;

nz=30;
n=nz-1;
d=4+(n-1)*2;
sn=[1:3;2:4];
tn=[1,4;2,3];
for m=2:n
    nm=(5+(m-2)*2):(6+(m-2)*2);
    c1=nm(1)-1;
    nc=[nm(1:end-1),c1;nm(2:end),nm(1)];
    sn=[sn,nc];
    tn=[tn,[nm(end);nm(1)]];
end

res=1e3;
kv=linspace(-pi/d12,pi/d12,res);
Ev=zeros(d,length(kv));

for m=1:length(kv)
    k=kv(m);
    i=[sn(1,:),sn(2,:),tn(1,:),tn(2,:)];
    j=[sn(2,:),sn(1,:),tn(2,:),tn(1,:)];
    v=[repmat(-t, 1,2*size(sn,2)), repmat(-t*exp(1i*k*d12),
    1,size(tn,2)), repmat(-t*exp(-1i*k*d12),1, size(tn,2))];

    hk=sparse(i,j,v,d,d);
    egv=eig(full(hk));
    Ev(:,m)=egv;
end

figure
plot(kv*d12,Ev/eV, 'b', 'LineWidth',1.5)
xlabel('k_y \rightarrow'); ylabel('E(k_y) in eV \rightarrow')
xticks([-2*pi -3*pi/2 -pi -pi/2 0 pi/2 pi 3*pi/2 2*pi]);
xticklabels({'-2\pi/d', '-3\pi/2d', '-\pi/d', '-\pi/2d', '0', '\pi/2d', '3\pi/2d', '2\pi/d'})
title(['ZGNR : Energy versus k_y fro N_z=', num2str(nz)])
```