Numerical Computations of Nanoelectronics Problems

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Outline
Three Lectures

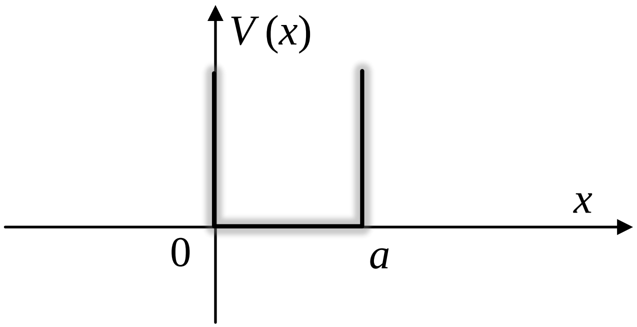
- Lecture on Tuesday
  - Numerical Calculation of Schrödinger Equation
    - 1D ∞ Quantum Well
  - Numerical Newton Iteration
    - Transcendental Equation (Capacitance of P-N Junction)
    - Poission's Equation (Band Diagram of P-N Junction)
- Lecture on Thursday
  - Numerical Calculation of Band Structures
    - 1D atom chain
    - Graphene Nanoribbon
    - Graphene
- Lecture in the final week
  - Quantum Transport – Non-equilibrium Green's Function

1D ∞ Quantum Well Numerical Calculation

- 1D ∞ Quantum Well

$$[H + V(x)]\psi = E\psi$$

$$H = -\frac{\hbar^2}{2m} \cdot \frac{d^2}{dx^2}$$



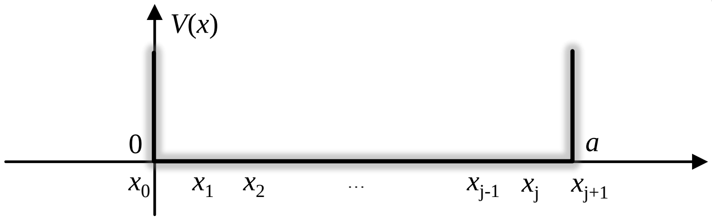
- Analytical Solution:

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}$$

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{a}} sin\left(\frac{n\pi x}{a}\right), & 0 < x < a \\ 0, & x < 0, x > a \end{cases}$$

1D ∞ Quantum Well Numerical Calculation

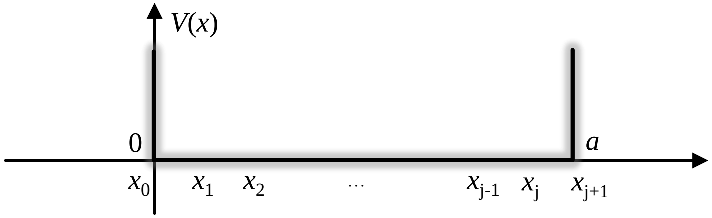
- Discretize the Problem:
- Wave Function



$$\psi_n(x) = \begin{pmatrix} \psi_n(x_1) \\ \psi_n(x_2) \\ \vdots \\ \vdots \\ \psi_n(x_l) \end{pmatrix} \qquad 0 = x_0 < x_j = \frac{j \cdot a}{l+1} < x_{l+1} = a, \qquad j = 1,2,\dots,l$$

$$\psi_n(x_0) = \psi_n(x_{l+1}) = 0$$

1D ∞ Quantum Well Numerical Calculation



- Discretize Hamiltonian

$$H = -\frac{\hbar^2}{2m} \cdot \frac{d^2}{dx^2}$$

$$\left.\frac{d^2}{dx^2}\psi_n\right|_{x=x_j} \approx \frac{1}{a/(l+1)}\left\{\frac{[\psi_n(x_{j+1}) - \psi_n(x_j)]}{a/(l+1)} - \frac{[\psi_n(x_j) - \psi_n(x_{j-1})]}{a/(l+1)}\right\}$$

$$= \left(\frac{l+1}{a}\right)^2 [\psi_n(x_{j+1}) - 2\psi_n(x_j) + \psi_n(x_{j-1})]$$

$$H\psi_n = -\frac{\hbar^2}{2m}\frac{(l+1)^2}{a^2}\begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & -2 \end{pmatrix}\begin{pmatrix} \psi_n(x_1) \\ \psi_n(x_2) \\ \vdots \\ \vdots \\ \psi_n(x_m) \end{pmatrix}$$

$$H = -\frac{\hbar^2}{2m}\frac{1}{a^2/(l+1)^2}\begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & -2 \end{pmatrix}$$

1D ∞ Quantum Well Numerical Calculation

- Solve in MATLAB

$$H = -\frac{\hbar^2}{2m}\frac{1}{a^2/(l+1)^2}\begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & -2 \end{pmatrix}$$

```
H=-h^2/2/m/a^2*(l+1)^2*...
   (diag(-2*ones(l,1))+...
    diag(ones(l-1,1),1) +...
    diag(ones(l-1,1),-1));
```

```
h=1.05e-34;
m=9.1e-31;
a=20e-10;
l=99;
e=1.6e-19;
```

1D ∞ Quantum Well Numerical Calculation

- Solve for eigenvalues and eigenvectors

```
[V,E]=eig(H);
```

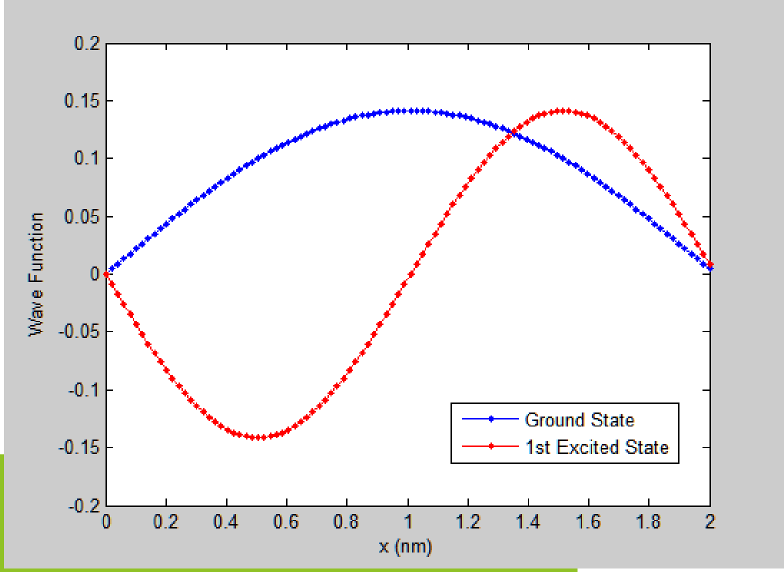
where

$$V = \left(\begin{bmatrix} \psi_1(x_1) \\ \psi_1(x_2) \\ \vdots \\ \psi_1(x_l) \end{bmatrix} \begin{bmatrix} \psi_2(x_1) \\ \psi_2(x_2) \\ \vdots \\ \psi_2(x_l) \end{bmatrix} \begin{bmatrix} \psi_l(x_1) \\ \psi_l(x_2) \\ \vdots \\ \psi_l(x_l) \end{bmatrix} \right)$$

$$E = \begin{pmatrix} E_1 & & \\ & \ddots & \\ & & E_l \end{pmatrix}$$

1D ∞ Quantum Well Numerical Calculation

- Check the results
- Wave Functions




```
figure;
hold on;box on;
axis([0 2 -0.2 0.2])
xlabel('x (nm)');
ylabel('Wave Function');
plot([0:l+1]*a/l*1e9,[0;V(:,1);0],'.-');
plot([0:l+1]*a/l*1e9,[0;V(:,2);0],'r.-');
legend('Ground State','1st Excited State');
```

1D ∞ Quantum Well Numerical Calculation

- Check the results
- Eigenvalues

```
diag(E)/e
```

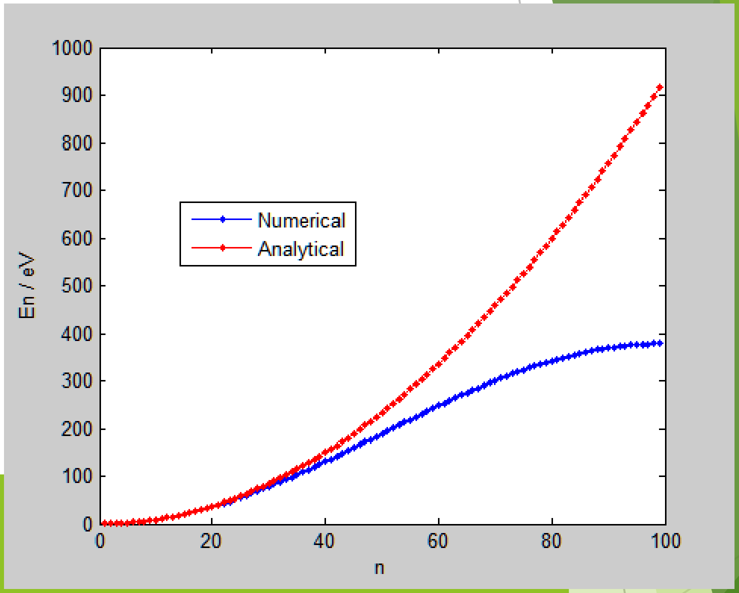
```
Command Window

>> diag(E)/e

ans =

    0.0934
    0.3735
    0.8401
    1.4927
    2.3306
    3.3531
    4.5590
    5.9473
```

```
figure;
hold on;box on;
xlabel('n');
ylabel('En / eV');
n=1:99;
plot(n,diag(E)/e,'.-');
plot(n,n.^2*h^2*pi^2/2/m/a^2/e,'r.-');
legend('Numerical','Analytical');
```

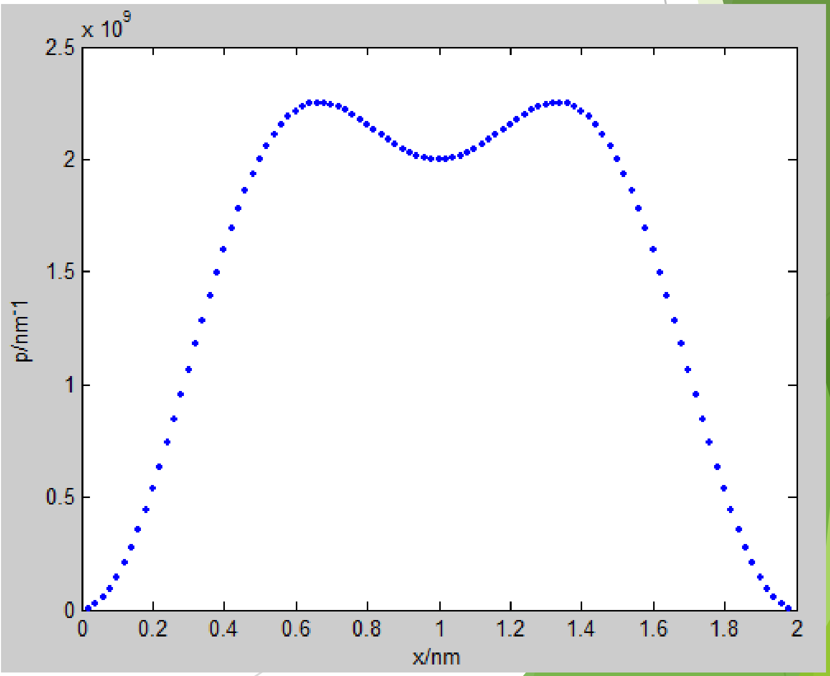


1D ∞ Quantum Well Numerical Calculation

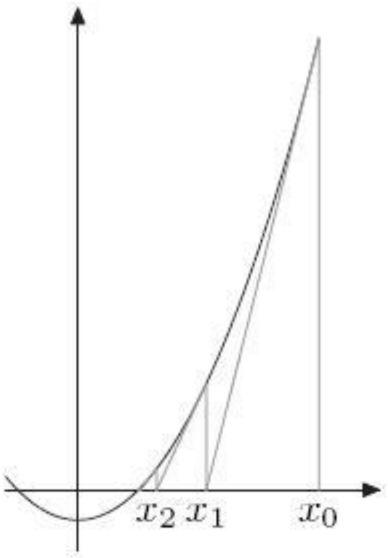
- Assignment 2, Problem 1:
- Use MATLAB to calculate the electron density in the well
- When Fermi level = E_2

$$\rho(x) = \sum_i N_i \psi_i^\dagger(x) \cdot \psi_i(x)$$

$$N_i = D_i \cdot f_{E_f}(E_i)$$



Newton Iteration (Newton's Method)



- To solve for the root of $f(x)$
- Steps:
- 1. Choose x_0 close to the root
- 2. $x_i = x_{i-1} - [f'(x_{i-1})]^{-1} f(x_{i-1}) \qquad i = 1,2,3,\dots$
- 3. Check the convergence condition

  $|x_i - x_{i-1}| < \eta$
- Yes → solved; No → return to step. 2

Newton Iteration Transcendental Equation

- Example:
- Solve the transcendental equantion below for V_{bi}

$$C' = \frac{C}{S} = \left[\frac{11.7 \cdot \varepsilon_0 e}{2(V_{bi} + V_R)} \frac{N_d N_a}{(N_a + N_d)}\right]^{\frac{1}{2}}$$

- Where $N_d = 9N_a$ $V_R = 1.2\ \mathrm{V}$ $C = 3.5\ \mathrm{pF}$ $S = 5.5 \times 10^{-4}\ \mathrm{cm}^{-2}$
- And V_{bi} can be yielded by Boltzmann approx.

$$V_{bi} = \frac{kT}{e} \ln\left(\frac{N_d N_a}{n_i^2}\right) = V_t \ln\left(\frac{N_d N_a}{n_i^2}\right)$$

Newton Iteration
Transcendental Equation

- $C' = \frac{C}{S} = \left[\frac{11.7 \cdot \varepsilon_0 e}{2(V_{bi} + V_R)} \frac{N_d N_a}{(N_a + N_d)}\right]^{\frac{1}{2}}$

- Use the given conditions, the equation becomes:

$$\left[\frac{11.7 \cdot \varepsilon_0 e}{2(V_{bi} + V_R)} \frac{3}{10} n_i \exp\left(\frac{V_{bi}}{2V_t}\right)\right]^{\frac{1}{2}} - C' = 0$$

- Find the zero of the function:

$$f(x) = \left[\frac{11.7 \cdot \varepsilon_0 e}{2(x + V_R)} \frac{3}{10} n_i \, exp\left(\frac{x}{2V_t}\right)\right]^{\frac{1}{2}} - C'$$

Newton Iteration Transcendental Equation

- First, derive for the derivative $f'(x)$ using MATLAB

```
global VR E0 Cp e ni Vt  %Constants
VR=1.2; E0=8.85*10^-14;
C=3.5*10^-12;S=5.5*10^-4;Cp=C/S;
e=1.6*10^-19;
ni=1.5*10^10;
Vt=0.0259;
syms x;
f=sqrt(11.7*E0*e*3*ni*... %f(x)
  exp(x/2/Vt)/(2*(x+VR)*10))-Cp;
fp=diff(f,'x')             %f' (x)
```

```
fp =
((3096785538529855625*exp((5000*x)/259))/(21516878181768325692630376788288077824*(20*x +
24)) - (24774284308238845*exp((5000*x)/259))/(166153499473114484112975882535043072*(20*x +
24)^2))/(2*((4954856861647769*exp((5000*x)/259))/(13292279957849158729038070602803445760*x
+ 15950735949418990474845684723364134912))^(1/2))
```

Newton Iteration Transcendental Equation

- Then build $f(x)$ and $f'(x)$ in MATLAB

```
function f=F(x)
    global VR E0 Cp e ni Vt
    f=sqrt(11.7*E0*e*3*ni*exp(x/2/Vt)/(2*(x+VR)*10))-Cp;
end
```

```
function fp=Fp(x);
    fp=1/2305843009213693952*99097137232955538^(1/2)...
    /(exp(5000/259*x)/(20*x+24))^(1/2)...*(5000/259...
    *exp(5000/259*x)/(20*x+24)-20*exp(5000/259*x)/(20*x+24)^2);
return
```

Newton Iteration
Transcendental Equation

- Start the iteration

```
x0=0.7;
x1=x0-F(x0)/Fp(x0)
x2=x1-F(x1)/Fp(x1)
x3=x2-F(x2)/Fp(x2)
```

x0 = 0.7
x1 = 0.6498
x2 = 0.6334
x3 = 0.6484
…

- When to end?

$$|x_i - x_{i-1}| < \eta$$

Newton Iteration Transcendental Equation

- Use loop

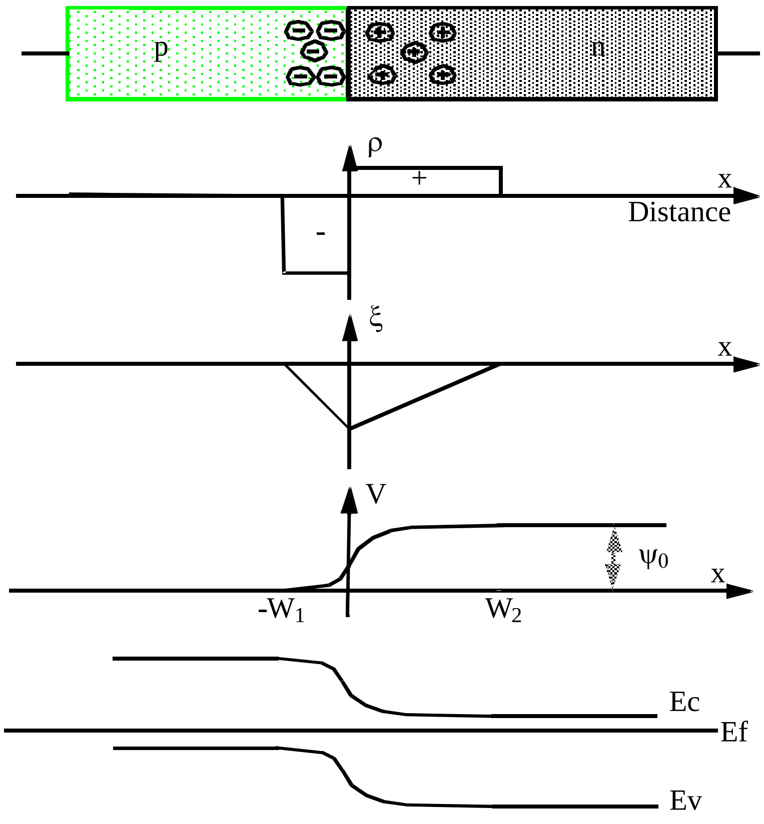
```
xi=0.7;          %Initial Value
ita=10^-10;      %Tolerance
while abs(xi-xim1)>ita
    xim1=xi;
    xi=xim1-F(xim1)/Fp(xim1);
end
Vbi=xi;
```

$$x_i = x_{i-1} - [f'(x_{i-1})]^{-1} f(x_{i-1})$$

Vbi = 0.6320
Na = 9.9513e+14
Nd = 8.9562e+15

Newton Iteration
Poisson's Equation

- Problem: Find the band diagram of a P-N Junction



(a) Schematic

(b) Charge density

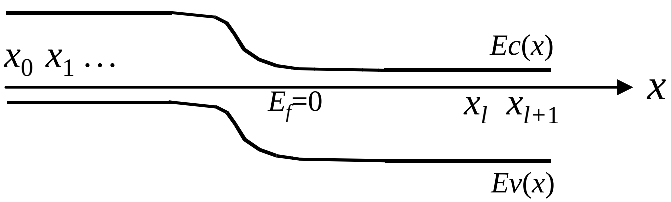
(c) Electric field.

(d) Electrostatic potential.

(e) Band Diagram

Newton Iteration Poisson's Equation

- Discretization



$$E_C(x) = \begin{pmatrix} E_C(x_1) \\ E_C(x_2) \\ \vdots \\ \vdots \\ E_C(x_l) \end{pmatrix} \qquad 0 = x_0 < x_j = \frac{j \cdot a}{l+1} < x_{l+1} = a$$

$$E_V(x) = E_C(x) - 1.12\ eV = \begin{pmatrix} E_V(x_1) \\ E_V(x_2) \\ \vdots \\ \vdots \\ E_V(x_l) \end{pmatrix}$$

$$\rho_{e,h}(x) = \begin{pmatrix} \rho(x_1) \\ \rho(x_2) \\ \vdots \\ \vdots \\ \rho(x_l) \end{pmatrix} \qquad \begin{aligned} \rho_e &= N_C\, exp\big((E_F - E_C)/kT\big) \\ \rho_h &= N_v\, exp(E_V - E_F)/kT\big) \end{aligned}$$

Newton Iteration
Poisson's Equation

- Consider Poisson's Equation:

$\nabla^2 U = Q/\epsilon$

- Transform into:

$\epsilon_{Si}\varepsilon_0\nabla^2(E_c/e) = e[N_d - N_a + \rho_h - \rho_e]$

$\epsilon_{Si} = 11.7,\ \varepsilon_0 = 8.85 \times 10^{-12}\,\mathrm{C}^2/(\mathrm{J}\cdot\mathrm{m})$

$$\epsilon_{Si}\varepsilon_0\nabla^2(E_C/e) = e\left[N_d - N_a + N_v\, exp\left(\frac{E_V - E_F}{kT}\right) - N_C\, exp\left(\frac{E_F - E_C}{kT}\right)\right]$$

$$f(E_C) = \epsilon_{Si}\varepsilon_0\nabla^2(E_C/e) - e\left[N_d + N_a - N_v\, exp\left(\frac{E_V - E_F}{kT}\right) + N_C\, exp\left(\frac{E_F - E_C}{kT}\right)\right]$$

Newton Iteration
Poisson's Equation

- Contd.

$$f(Ec) = \varepsilon_{si}\varepsilon_0 \nabla^2 \frac{Ec}{e} + e\left[-N_d + N_a - N_v \exp(\frac{Ev - Ef}{kT}) + N_c \exp(\frac{Ef - Ec}{kT})\right]$$

$$f(Ec) = \frac{\varepsilon_{si}\varepsilon_0}{e} \nabla^2 Ec + e\left[-N_d + N_a - N_v \exp(\frac{Ec - Eg}{kT}) + N_c \exp(\frac{Ef - Ec}{kT})\right]$$

- How to discretize it?
- Recall

$$H\psi_n = -\frac{\hbar^2}{2m}\frac{(l+1)^2}{a^2}\begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & -2 \end{pmatrix}\begin{pmatrix} \psi_n(x_1) \\ \psi_n(x_2) \\ \vdots \\ \vdots \\ \psi_n(x_m) \end{pmatrix}$$

Newton Iteration
Poisson's Equation

- Boundary Conditions $\left.\frac{\partial E_C}{\partial x}\right|_{x=0,a} = 0$

- Laplacian Operator

$$\nabla^2 = \frac{(l+1)^2}{a^2}\begin{bmatrix} -1 & 1 & & & \\ 1 & -2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & -2 & 1 \\ & & & 1 & -1 \end{bmatrix}$$

$$\nabla^2 Ec = \frac{(l+1)^2}{a^2}\begin{bmatrix} -1 & 1 & & & \\ 1 & -2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & -2 & 1 \\ & & & 1 & -1 \end{bmatrix}\begin{bmatrix} Ec(x_1) \\ Ec(x_2) \\ . \\ . \\ Ec(x_L) \end{bmatrix}$$

$$f(Ec) = \varepsilon_{si}\varepsilon_0 \frac{(l+1)^2}{ea^2}\begin{bmatrix} -1 & 1 & & & \\ 1 & -2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & -2 & 1 \\ & & & 1 & -1 \end{bmatrix} Ec$$

$$+ e\left[-N_d + N_a - N_v \exp\left(\frac{Ec - Eg}{kT}\right) + N_c \exp\left(\frac{Ef - Ec}{kT}\right) \right]$$

Newton Iteration
Poisson's Equation

- $$N_d = \begin{bmatrix} N_d(x_1) \\ N_d(x_2) \\ . \\ . \\ N_d(x_j) \end{bmatrix} \quad N_a = \begin{bmatrix} N_a(x_1) \\ N_a(x_2) \\ . \\ . \\ N_a(x_j) \end{bmatrix}$$

- Discrete Poisson's Equation for P-N Junction:

$$f(Ec) = \varepsilon_{si}\varepsilon_0 \frac{(l+1)^2}{ea^2} \begin{bmatrix} -1 & 1 & & & \\ 1 & -2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & -2 & 1 \\ & & & 1 & -1 \end{bmatrix} \begin{bmatrix} Ec(x_1) \\ Ec(x_2) \\ . \\ . \\ Ec(x_j) \end{bmatrix}$$

$$+e\left[-\begin{bmatrix} N_d(x_1) \\ N_d(x_2) \\ . \\ . \\ N_d(x_j) \end{bmatrix} + \begin{bmatrix} N_a(x_1) \\ N_a(x_2) \\ . \\ . \\ N_a(x_j) \end{bmatrix} - N_v \exp(\begin{bmatrix} Ec(x_1)-Eg \\ Ec(x_2)-Eg \\ . \\ . \\ Ec(x_j)-Eg \end{bmatrix} / kT) + N_c \exp(Ef - \begin{bmatrix} Ec(x_1) \\ Ec(x_2) \\ . \\ . \\ Ec(x_j) \end{bmatrix} / kT) \right]$$

```
global Es Eo kT e Nc Nv Eg l a Nd Na diagm  %Constants
Es=11.7; Eo=8.85e-14; e=1.6e-19; kT=0.0259*e;
Nc=2.8e19; Nv=1.04e19; Eg=1.12*e;Ef=0;
l=99; a=10^-4;
Nd=[ones((l+1)/2,1)*1e16;  zeros((l-1)/2,1)];      %Doping profile
Na=[zeros((l+1)/2,1);  ones((l-1)/2,1)*1e16];
diagm=(diag(-2*ones(l,1))+diag(ones(l-1,1),1)+diag(ones(l-1,1),-1));
diagm(1,1)=-1;
diagm(l,l)=-1;      % Laplacian Matrix
```

$$f(Ec) = \varepsilon_{si}\varepsilon_0 \frac{(l+1)^2}{ea^2} \begin{bmatrix} -1 & 1 & & & \\ 1 & -2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & -2 & 1 \\ & & & 1 & -1 \end{bmatrix} \begin{bmatrix} Ec(x_1) \\ Ec(x_2) \\ . \\ . \\ Ec(x_j) \end{bmatrix}$$

$$+e\left[-\begin{bmatrix} N_d(x_1) \\ N_d(x_2) \\ . \\ . \\ N_d(x_j) \end{bmatrix} + \begin{bmatrix} N_a(x_1) \\ N_a(x_2) \\ . \\ . \\ N_a(x_j) \end{bmatrix} - N_v \exp\left(\begin{bmatrix} Ec(x_1)-Eg \\ Ec(x_2)-Eg \\ . \\ . \\ Ec(x_j)-Eg \end{bmatrix} / kT \right) + N_c \exp\left(Ef - \begin{bmatrix} Ec(x_1) \\ Ec(x_2) \\ . \\ . \\ Ec(x_j) \end{bmatrix} / kT \right) \right]$$

```
f=Eo*Es/e*((l+1)^2/a^2)*diagm*Ec...
  +e*(-Nd+Na-Nv*exp((Ec-Eg)/kT)+Nc*exp((Ef-Ec)/kT));
```

Newton Iteration
Poisson's Equation

- Newton's Method for $y = f(x)$: $x_i = x_{i-1} - [f'(x_{i-1})]^{-1} f(x_{i-1})$
- Newton's Method for vector function?

$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}, \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} f_1(\boldsymbol{x}) \\ f_2(\boldsymbol{x}) \\ \vdots \\ f_n(\boldsymbol{x}) \end{pmatrix}$$

- Jacobi Matrix

$$\mathbf{J} = \frac{\partial f}{\partial \boldsymbol{x}} = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_j} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_j} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \ddots & & & \vdots \\ \frac{\partial f_i}{\partial x_1} & \frac{\partial f_i}{\partial x_2} & & \frac{\partial f_i}{\partial x_j} & & \frac{\partial f_i}{\partial x_n} \\ \vdots & \vdots & & & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_j} & \cdots & \frac{\partial f_n}{\partial x_n} \end{pmatrix}$$

$$\boldsymbol{x}_{i+1} = \boldsymbol{x}_i - \left(\frac{\partial f}{\partial \boldsymbol{x}}\right)^{-1} f(\boldsymbol{x}_i)$$

$$f(Ec)=\varepsilon_{si}\varepsilon_0\frac{(l+1)^2}{ea^2}\begin{bmatrix}-1 & 1 & & & \\ 1 & -2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & -2 & 1 \\ & & & 1 & -1\end{bmatrix}\begin{bmatrix}Ec(x_1)\\ Ec(x_2)\\ .\\ .\\ Ec(x_j)\end{bmatrix}$$

$$+e\left[-\begin{bmatrix}N_d(x_1)\\ N_d(x_2)\\ .\\ .\\ N_d(x_j)\end{bmatrix}+\begin{bmatrix}N_a(x_1)\\ N_a(x_2)\\ .\\ .\\ N_a(x_j)\end{bmatrix}-N_v\exp(\begin{bmatrix}Ec(x_1)-Eg\\ Ec(x_2)-Eg\\ .\\ .\\ Ec(x_j)-Eg\end{bmatrix}/kT)+N_c\exp(Ef-\begin{bmatrix}Ec(x_1)\\ Ec(x_2)\\ .\\ .\\ Ec(x_j)\end{bmatrix}/kT)\right]$$

$$J=\varepsilon_{si}\varepsilon_0\frac{(l+1)^2}{ea^2}\begin{bmatrix}-1 & 1 & & & \\ 1 & -2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & -2 & 1 \\ & & & 1 & -1\end{bmatrix}$$

$$-\frac{eN_v}{kT}\begin{bmatrix}\exp(\frac{Ec(x_1)-Eg}{kT}) & & & & \\ & \cdots & & & \\ & & \exp(\frac{Ec(x_i)-Eg}{kT}) & & \\ & & & \cdots & \\ & & & & \exp(\frac{Ec(x_L)-Eg}{kT})\end{bmatrix}$$

$$-\frac{eN_c}{kT}\begin{bmatrix}\exp(\frac{Ef-Ec(x_1)}{kT}) & & & & \\ & \cdots & & & \\ & & \exp(\frac{Ef-Ec(x_i)}{kT}) & & \\ & & & \cdots & \\ & & & & \exp(\frac{Ef-Ec(x_L)}{kT})\end{bmatrix}$$

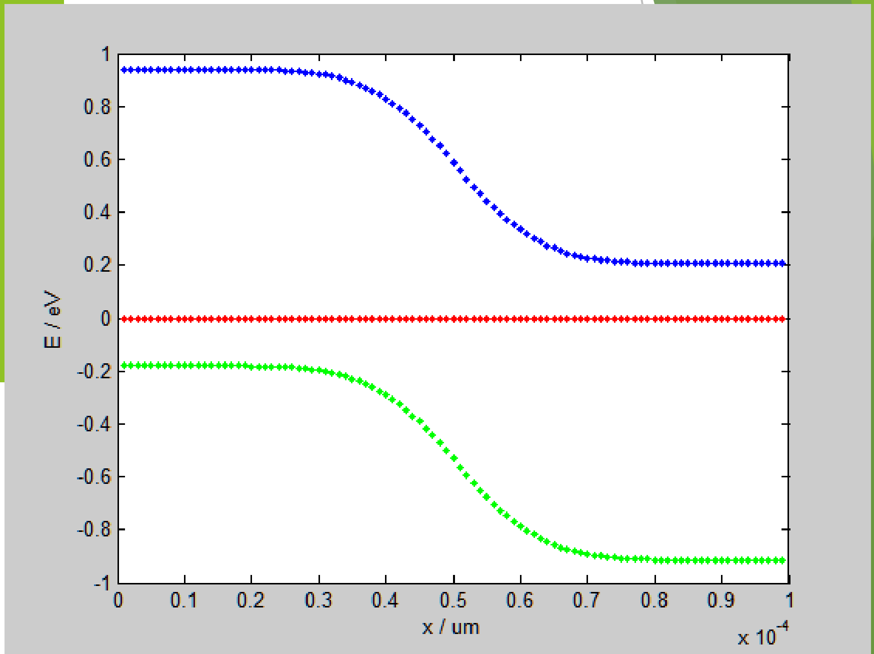
$$J=\varepsilon_{si}\varepsilon_0\frac{(l+1)^2}{ea^2}\begin{bmatrix}-1 & 1 & & & \\ 1 & -2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & -2 & 1 \\ & & & 1 & -1\end{bmatrix}$$

$$-\frac{eN_v}{kT}\begin{bmatrix}\exp(\frac{Ec(x_1)-Eg}{kT}) & & & & \\ & \cdots & & & \\ & & \exp(\frac{Ec(x_i)-Eg}{kT}) & & \\ & & & \cdots & \\ & & & & \exp(\frac{Ec(x_L)-Eg}{kT})\end{bmatrix}$$

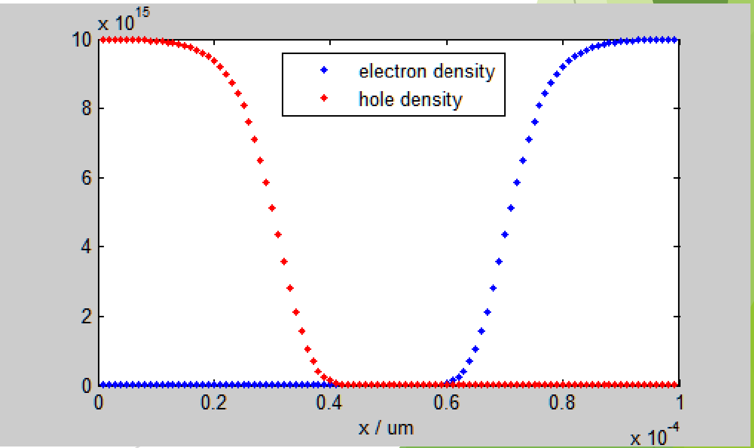
$$-\frac{eN_c}{kT}\begin{bmatrix}\exp(\frac{Ef-Ec(x_1)}{kT}) & & & & \\ & \cdots & & & \\ & & \exp(\frac{Ef-Ec(x_i)}{kT}) & & \\ & & & \cdots & \\ & & & & \exp(\frac{Ef-Ec(x_L)}{kT})\end{bmatrix}$$

```
J=Es*Eo/e*((l+1)^2)/(a^2)*diagm-e*Nv/kT*diag(exp((Ec-Eg)/kT))-e*Nc/kT*diag(exp((Ef-Ec)/kT));
```

```
Ec=zeros(l,1);      %Initial value
ita=10^-8;          %Tolerance
delta=1;            %difference
while delta>ita
    f=F(Ec);
    J=J(Ec); %Jacobi
    Ecp=Ec-J\f;
    delta=max(abs(Ec-Ecp))/e;
    Ec=Ecp;
end
```

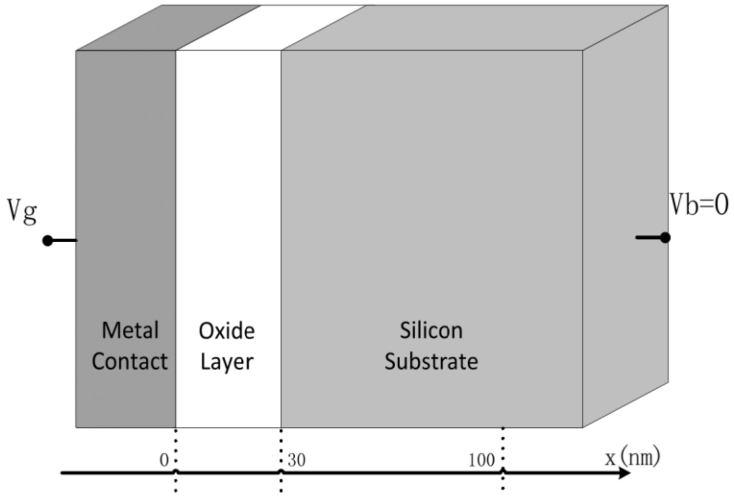


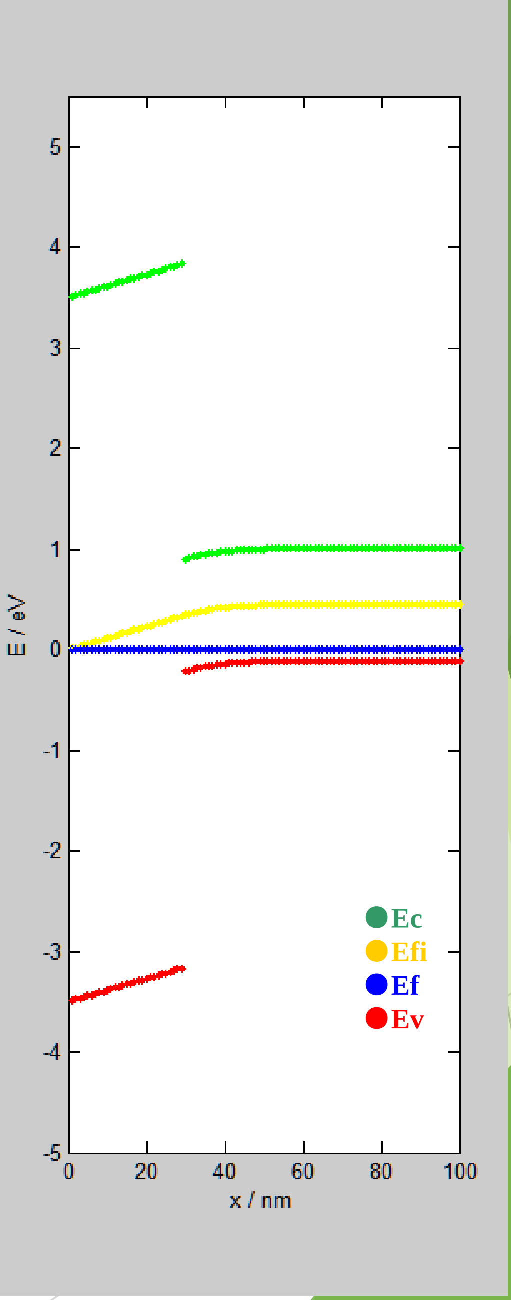

```
hold on;
box on;
xlabel('x / um');
ylabel('E / eV');
plot([1:l]*a/(l+1),Ec/e,'.-');
plot([1:l]*a/(l+1),Ef/e,'r.-');
plot([1:l]*a/(l+1),Ec/e-Eg/e,'g.-');
```



Newton Iteration
Poisson's Equation

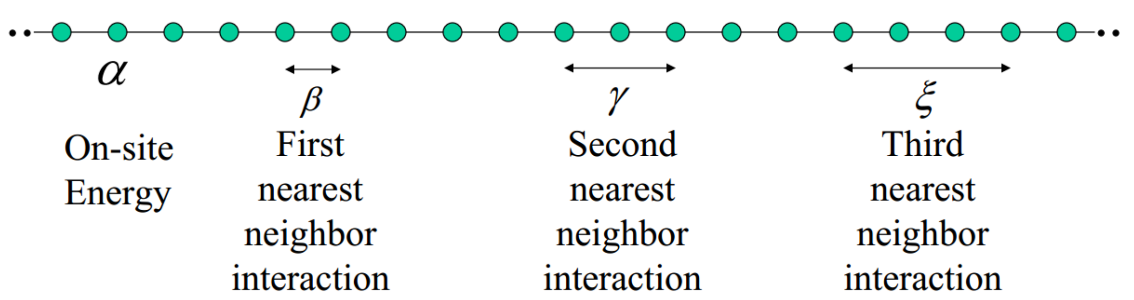
- Assignment 2, Problem 2:
- Use MATLAB to calculate the band structure of a MOS capacitor





Band Structures
Tight-Binding Method

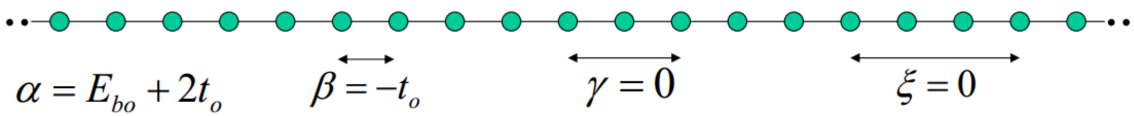
- TB description for 1D chain of atoms



$$H = \begin{bmatrix} \alpha & \beta & \gamma & \xi & . \\ \beta^{+} & \alpha & \beta & \gamma & . \\ \gamma^{+} & \beta^{+} & \alpha & \beta & . \\ \xi^{+} & \gamma^{+} & \beta^{+} & \alpha & . \\ . & . & . & . & \ldots \end{bmatrix}$$

Band Structures
Tight-Binding Method

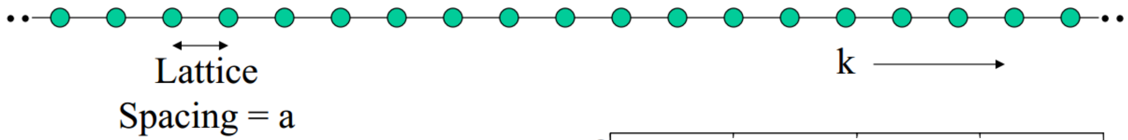
- First Nearest Neighbor TB Description



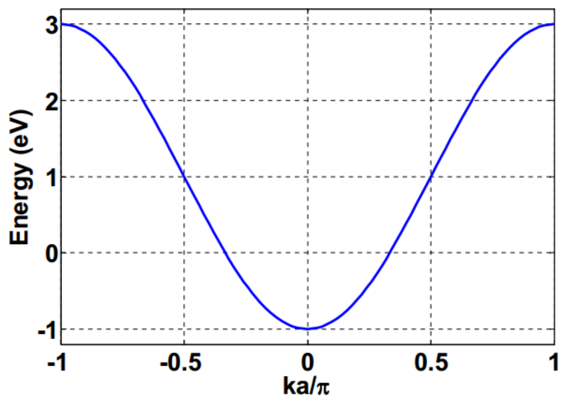
$$H = \begin{bmatrix} E_{bo}+2t_o & -t_o & 0 & 0 & . \\ -t_o & E_{bo}+2t_o & -t_o & 0 & . \\ 0 & -t_o & E_{bo}+2t_o & -t_o & . \\ 0 & 0 & -t_o & E_{bo}+2t_o & . \\ . & . & . & . & \cdots \end{bmatrix}$$

Band Structures
Tight-Binding Method

- First Nearest Neighbor TB Description – E(k)



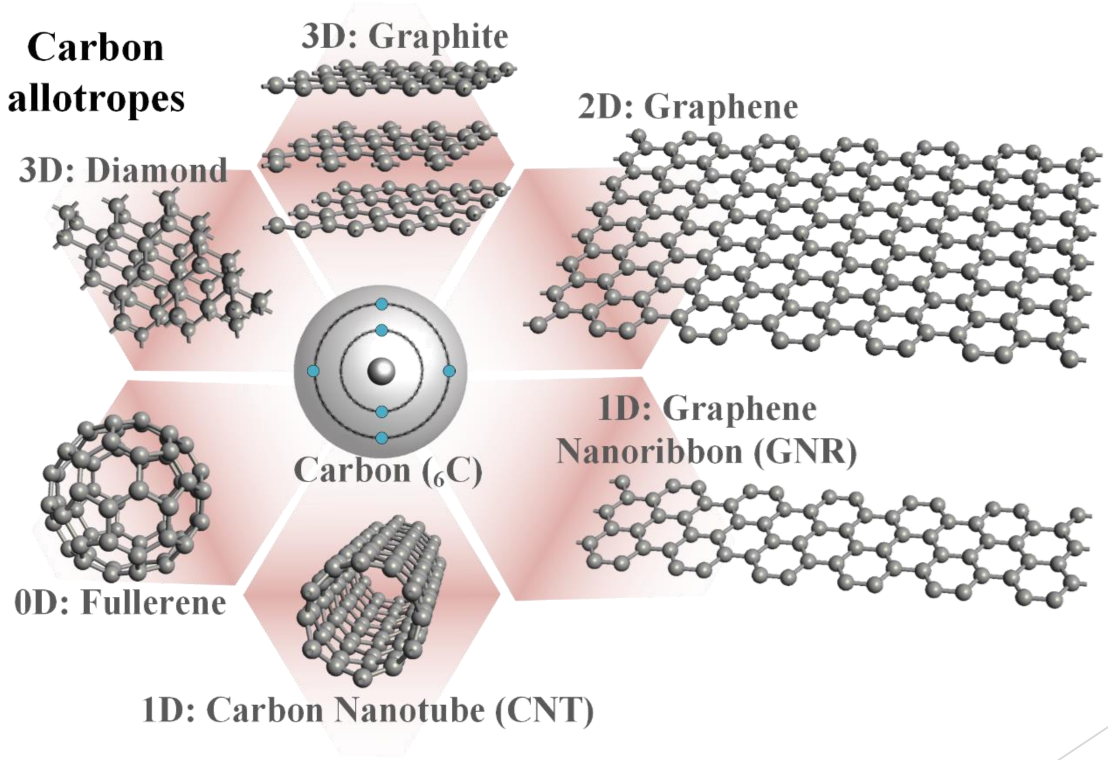
$$E(k) = \sum_{m=1}^{N} H_{mn} e^{i\vec{k}.(\vec{d_m} - \vec{d_n})}$$
$$= E_{bo} + 2t_o - t_o e^{ika} - t_o e^{-ika}$$
$$= E_{bo} + 2t_o - t_o \left[e^{ika} + e^{-ika} \right]$$
$$= E_{bo} + 2t_o \left[1 - \cos(ka) \right]$$



- Applications:
  - effective mass model for various materials
  - pz-orbital tight binding model for CNTs and GNRs.

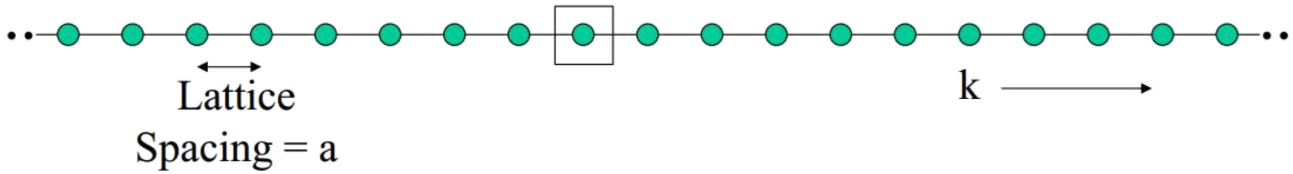
Band Structures
Tight-Binding Method

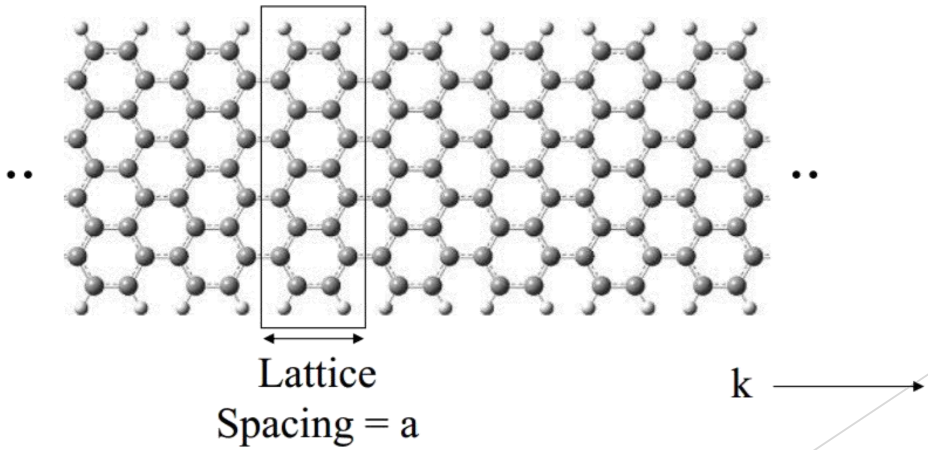
- Graphene Nanoribbon



Band Structures
Tight-Binding Method

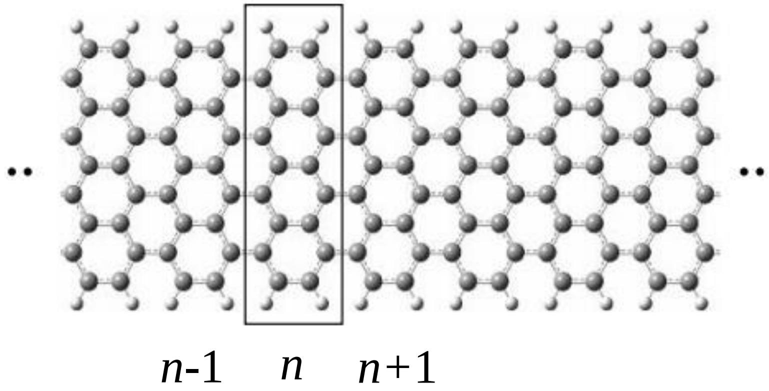
- Problem: Band structure of GNR





Band Structures
Tight-Binding Method

- $$E(k)=\sum_{m=1}^{N} H_{mn} e^{i\vec{k}.(\vec{d_m}-\vec{d_n})}$$



$$H_{n,n}$$

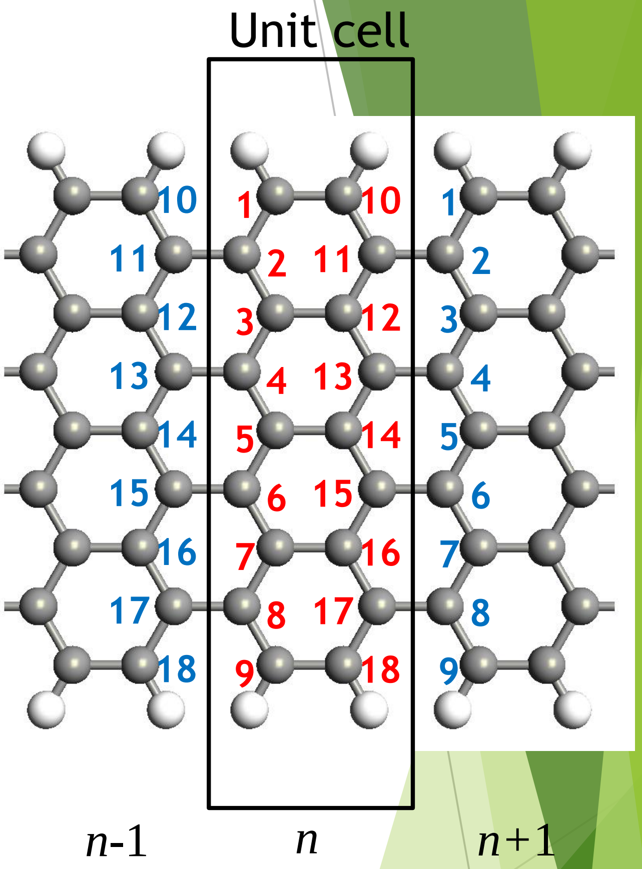
$$H_{n,n+1}$$

$$H_{n,n-1}$$

- Hamiltonian

H_{nn} =

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1		t								t								
2	t		t															
3		t		t								t						
4			t		t													
5				t		t								t				
6					t		t											
7						t		t								t		
8							t		t									
9								t										t
10	t										t							
11										t		t						
12			t								t		t					
13												t		t				
14					t								t		t			
15														t		t		
16							t								t		t	
17																t		t
18									t								t	




```
t=2.7;
Hnn_ul=diag(ones(8,1),1)+diag(ones(8,1),-1);
Hnn_br=diag(ones(8,1),1)+diag(ones(8,1),-1);
Hnn_ur=diag([1 0 1 0 1 0 1 0 1]);
Hnn_bl=diag([1 0 1 0 1 0 1 0 1]);
Hnn=t*[Hnn_ul Hnn_ur; Hnn_bl Hnn_br];
```

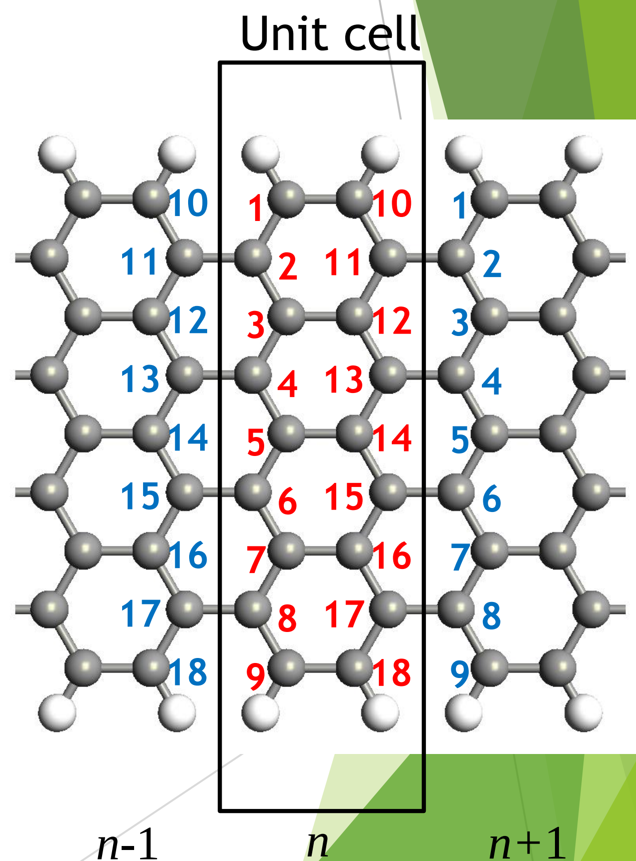
Band Structures
Tight-Binding Method

- Hamiltonian

$H_{n,n+1} =$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1																		
2																		
3																		
4																		
5																		
6																		
7																		
8																		
9																		
10																		
11		t																
12																		
13				t														
14																		
15						t												
16																		
17								t										
18																		

```
Hnm=t*diag([0 1 0 1 0 1 0 1 0], 9);
```



Band Structures
Tight-Binding Method

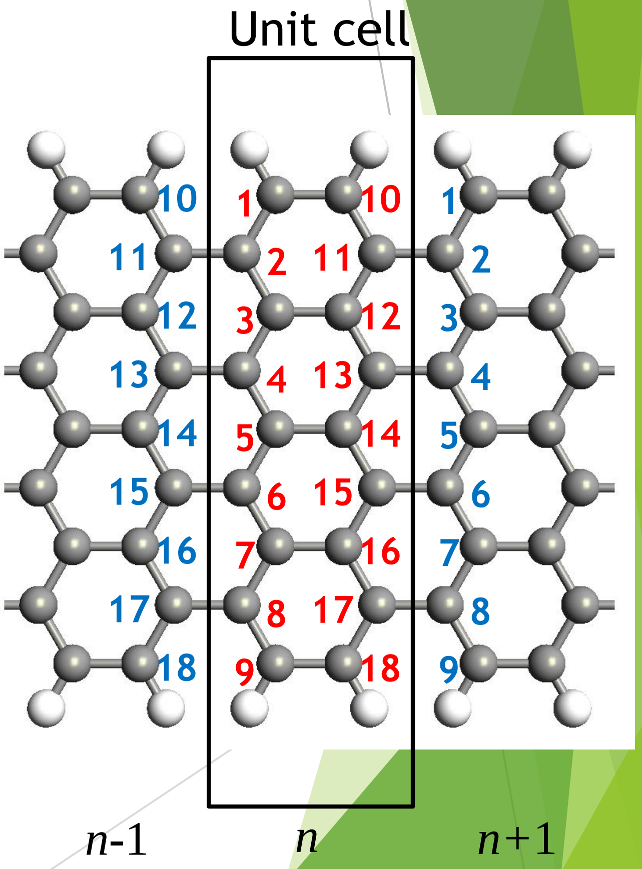
- Hamiltonian

$H_{n,n-1} =$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1																		
2											t							
3																		
4													t					
5																		
6															t			
7																		
8																	t	
9																		
10																		
11																		
12																		
13																		
14																		
15																		
16																		
17																		
18																		

```
Hmn=t*diag([0 1 0 1 0 1 0 1 0], -9);
```

transpose of $H_{n,n+1}$



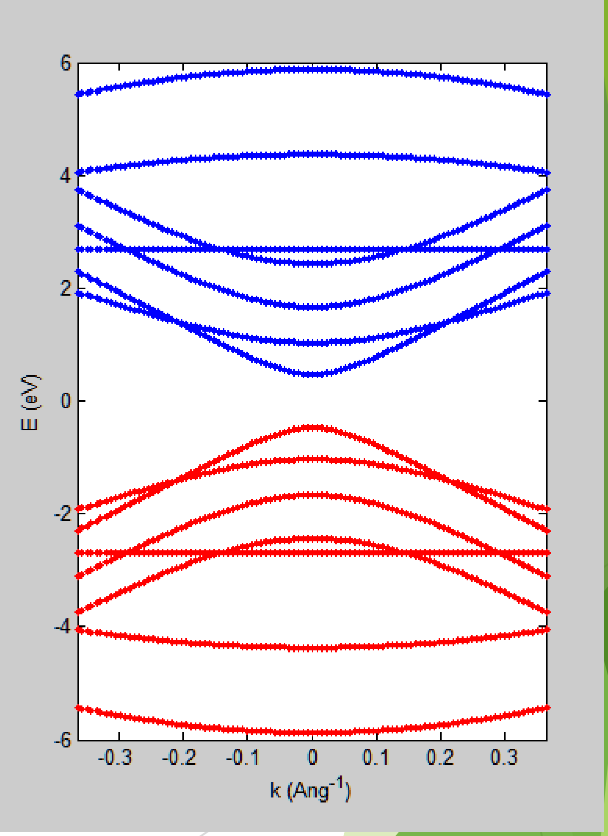
Band Structures
Tight-Binding Method

- Hamiltonian:

$$\sum_{m=1}^{N} H_{mn} e^{i\vec{k}.(\vec{d}_m - \vec{d}_n)}$$

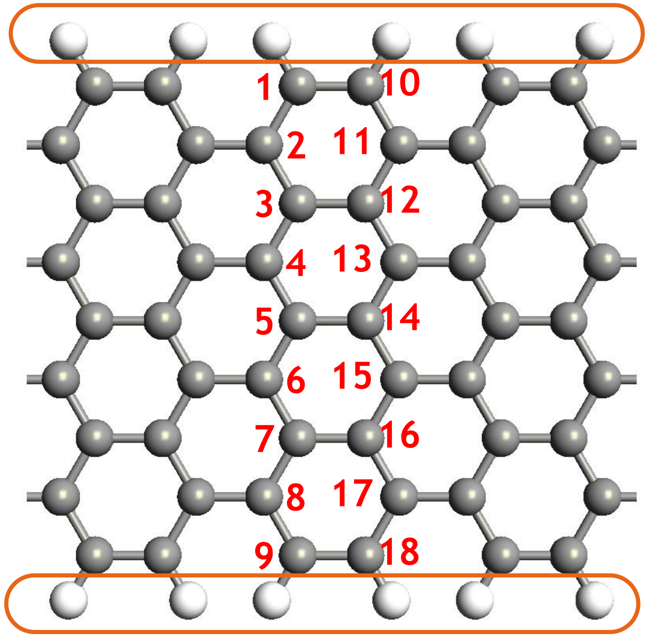
$$= H_{nn} + H_{n,n+1}e^{-ika} + H_{n,n-1}e^{ika}$$

```
hold on; box on;
a=3*1.44;
k_grid=linspace(-pi/2/a,pi/2/a,101);
for k=k_grid
    H=Hnn+Hnm*exp(-1i*k*a)+Hmn*exp(1i*k*a);
    [V E]=eig(H);
    E=diag(E);
    plot(k,E(1:9),'r.');
    plot(k,E(10:18),'b.');
end
axis tight
ylim([-6 6]);
xlabel('k (Ang^{-1})');
ylabel('E (eV)');
```



Band Structures
Tight-Binding Method

- Considering hydrogen atoms at edges…

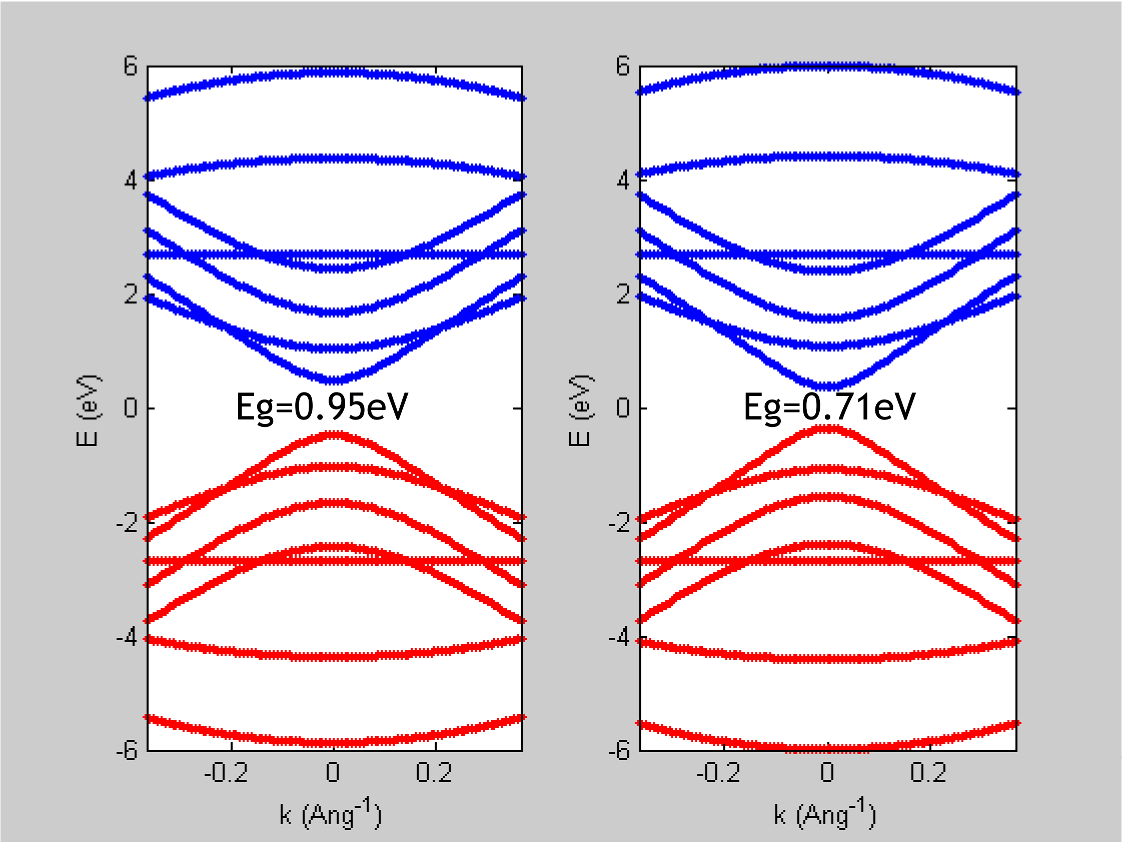


$H_{nn} =$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1		t								$t \times 1.12$								
2	t		t															
3		t		t								t						
4			t		t													
5				t		t								t				
6					t		t											
7						t		t								t		
8							t		t									
9								t										$1.12 \times t$
10	$t \times 1.12$										t							
11										t		t						
12			t								t		t					
13												t		t				
14					t								t		t			
15														t		t		
16							t								t		t	
17																t		t
18									$t \times 1.12$								t	

```
Hnm=t*diag([0 1.12 0 1 0 1 0 1.12 0], 9);
Hmn=t*diag([0 1.12 0 1 0 1 0 1.12 0], -9);
```

Band Structures
Tight-Binding Method

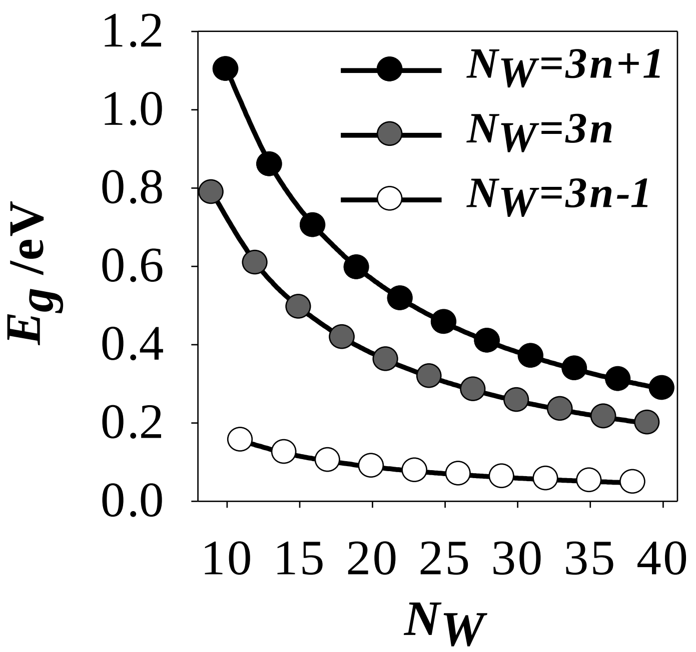


Unsaturated

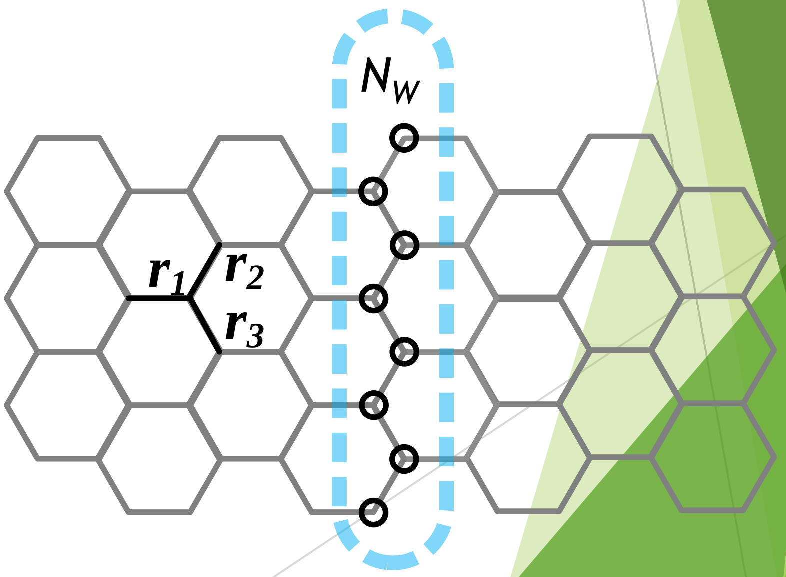
Hydrogen saturated

Band Structures
Tight-Binding Method

- Armchair GNR Band gap – TB Results

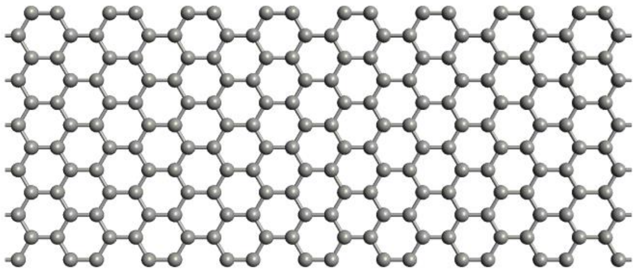


N_W=number of C atom along width

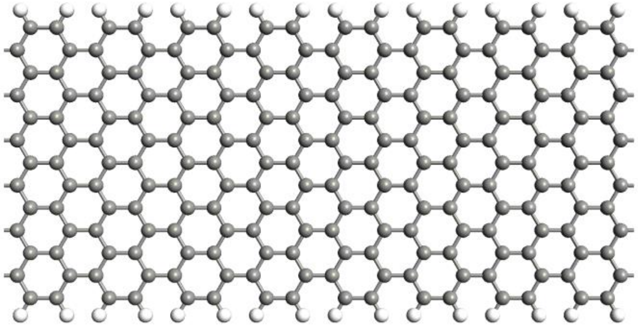


Band Structures
Tight-Binding Method

- Assignment 2, Problem 4:
- Calculate GNR band structure for:



N_W=12 unsaturated edge



N_W=13 saturated edge

Band Structures
Tight-Binding Method

- Band structure of graphene?

$$H = H_{nn} + H_{n,n1}e^{-i\vec{k}\overrightarrow{a1}} + H_{n,n2}e^{-i\vec{k}\overrightarrow{a2}} + H_{n,n3}e^{-i\vec{k}\overrightarrow{a3}} + H_{n,n4}e^{-i\vec{k}\overrightarrow{a4}}$$

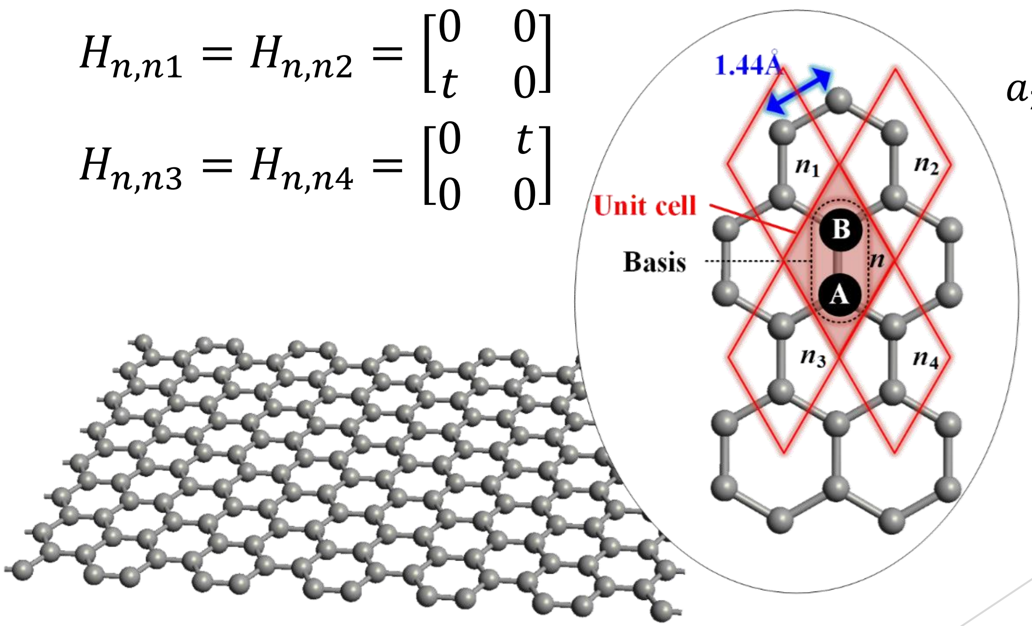
$$H_{nn} = \begin{bmatrix} 0 & t \\ t & 0 \end{bmatrix}$$

$$H_{n,n1} = H_{n,n2} = \begin{bmatrix} 0 & 0 \\ t & 0 \end{bmatrix}$$

$$H_{n,n3} = H_{n,n4} = \begin{bmatrix} 0 & t \\ 0 & 0 \end{bmatrix}$$

$$a_1 = -a_3 = 1.44\text{Å} \times \left(\frac{3}{2}, \frac{\sqrt{3}}{2}\right)$$

$$a_2 = -a_4 = 1.44\text{Å} \times \left(\frac{3}{2}, -\frac{\sqrt{3}}{2}\right)$$



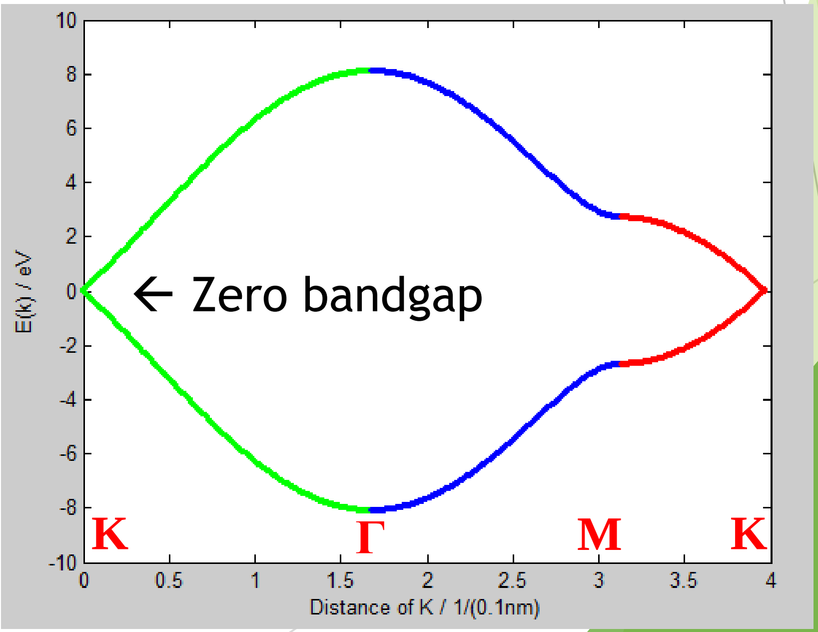
Band Structures
Tight-Binding Method

- Solve *H* in MATLAB along the route

$$k=(0\,,0\,,0)\rightarrow k=(\frac{2\pi}{3a_{cc}}\,,0\,,0)\rightarrow k=(\frac{2\pi}{3a_{cc}}\,,\frac{2\pi}{3\sqrt{3}a_{cc}}\,,0)$$

Symmetric point **Γ** in k space

K **M**



Band Structures Tight-Binding Method

- Solve in k plane:
- Assignment 2 Bonus Problem: plot this figure using MATLAB