MATLAB codes used to generate text figures

Chapter 1

% Fig.1.1.1

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;q=1.602e-19;eps0=8.854E-12;epsr=4;m=0.25*9.11e-31;%Effective mass
I0=q*q/hbar;

%Parameters
W=1e-6;L=10e-9;t=1.5e-9;%W=Width,L=Length of active region,t=oxide thickness
Cg=epsr*eps0*W*L/t;Cs=0.05*Cg;Cd=0.05*Cg;CE=Cg+Cs+Cd;U0=q/CE;
alphag=Cg/CE,alphad=Cd/CE
    %alphag=1;alphad=0.5;U0=0.25;

kT=0.025;mu=0;ep=0.2;
    v=1e5;%Escape velocity
        g1=hbar*v/(q*L);g2=g1;g=g1+g2;
            %g1=0.005;g2=0.005;g=g1+g2;

%Energy grid
NE=501;E=linspace(-1,1,NE);dE=E(2)-E(1);
    D0=m*q*W*L/(pi*hbar*hbar);% Step Density of states per eV
    D=D0*[zeros(1,251) ones(1,250)];
    %D=(2*g/(2*pi))./((E.^2)+((g/2)^2));% Lorentzian Density of states per eV
        %D=D./(dE*sum(D));%Normalizing to one

%Reference number of electrons
f0=1./(1+exp((E+ep-mu)./kT));N0=2*dE*sum(D.*f0);ns=N0/(L*W*1e4),%/cm^2

%Bias
IV=61;VV=linspace(0,0.6,IV);
for iV=1:IV
    Vg=0.5;Vd=VV(iV);
```

```
    %Vd=0.5;Vg=VV(iV);
        mu1=mu;mu2=mu1-Vd;UL=-(alphag*Vg)-(alphad*Vd);

U=0;%Self-consistent field
dU=1;
while dU>1e-6
    f1=1./(1+exp((E+UL+U+ep-mu1)./kT));
        f2=1./(1+exp((E+UL+U+ep-mu2)./kT));
    N(iV)=dE*sum(D.*((f1.*g1/g)+(f2.*g2/g)));
        Unew=U0*(N(iV)-N0);dU=abs(U-Unew);
            U=U+0.1*(Unew-U);
end
I(iV)=dE*I0*(sum(D.*(f1-f2)))*g1*g2/g;
end

hold on
h=plot(VV,I,'b');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[25])
xlabel(' Voltage (V) --->')
ylabel(' Current (A) ---> ')
grid on
```

% Fig.1.1.3

```
clear all

E=linspace(-.25,.25,501);dE=E(2)-E(1);kT=0.025;Ef=0;
V=0;mu1=Ef+(V/2);mu2=Ef-(V/2);
f1=1./(1+exp((E-mu1)./kT));f2=1./(1+exp((E-mu2)./kT));
%dE*(sum(f1-f2))/V

hold on
h=plot(f1,E,'g');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[25])
xlabel(' Fermi function --->')
ylabel(' E - mu (eV) ---> ')
grid on
```

% Fig.1.3.3, 1.5.1

```
clear all

E=linspace(-.5,.5,50001);dE=E(2)-E(1);gam=0.05;
D=(gam/(2*pi))./((E.^2)+((gam/2)^2));
%D=(gam/(2*pi))./(((E-0.25).^2)+((gam/2)^2));%Use for Fig.1.5.2
%D=D+((gam/(2*pi))./(((E+0.25).^2)+((gam/2)^2)));%Use for Fig.1.5.2
dE*sum(D)

hold on
h=plot(D,E,'g');
```

```
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[25])
xlabel(' D (E) --->')
ylabel(' E (eV) ---> ')
grid on
```

% Fig.1.4.6

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;q=1.602e-19;I0=q*q/hbar;

%Parameters
U0=0.025;kT=0.025;mu=0;ep=0.2;
g1=0.005;g2=0.005;g=g1+g2;
alphag=1;alphad=0.5;

%Energy grid
NE=501;E=linspace(-1,1,NE);dE=E(2)-E(1);
D=(g/(2*pi))./((E.^2)+((g/2)^2));% Lorentzian Density of states per eV
D=D./(dE*sum(D));%Normalizing to one

%Bias
IV=101;VV=linspace(0,1,IV);
for iV=1:IV
    Vg=0;Vd=VV(iV);
    %Vd=0;Vg=VV(iV);
        mu1=mu;mu2=mu1-Vd;UL=-(alphag*Vg)-(alphad*Vd);

U=0;%Self-consistent field
dU=1;
while dU>1e-6
    f1=1./(1+exp((E+ep+UL+U-mu1)./kT));
        f2=1./(1+exp((E+ep+UL+U-mu2)./kT));
    N(iV)=dE*sum(D.*((f1.*g1/g)+(f2.*g2/g)));
        Unew=U0*N(iV);dU=abs(U-Unew);
            U=U+0.1*(Unew-U);
end
I(iV)=dE*I0*(sum(D.*(f1-f2)))*(g1*g2/g);
end

hold on
h=plot(VV,N,'b');
%h=plot(VV,I,'b');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[25])
xlabel(' Voltage ( V ) --->')
%ylabel(' Current ( A ) ---> ')
ylabel(' Number of electrons ---> ')
grid on
```

% Fig.E.1.3

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;q=1.602e-19;I0=q*q/hbar;

%Parameters
U0=0.025;kT1=0.026;kT2=0.025;ep=0.2;
g1=0.005;g2=0.005;g=g1+g2;
alphag=1;alphad=0.5;

%Energy grid
NE=501;E=linspace(-1,1,NE);dE=E(2)-E(1);
g1=0.005*(E+abs(E))./(E+E+1e-6);% zero for negative E
g2=0.005*ones(1,NE);g1=g2;
g=g1+g2;

%Bias
IV=101;VV=linspace(-0.25,0.25,IV);
for iV=1:IV
      mu1=ep+VV(iV);mu2=mu1;
            f1=1./(1+exp((E-mu1)./kT1));
            f2=1./(1+exp((E-mu2)./kT2));
            D=(g./(2*pi))./(((E-ep).^2)+((g./2).^2));
                  D=D./(dE*sum(D));
I(iV)=dE*2*I0*(sum(D.*(f1-f2).*g1.*g2./g));
end

hold on
%h=plot(VV,N/2,'b');%Part (a)
h=plot(VV,I,'b');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[25])
xlabel(' Voltage ( V ) --->')
ylabel(' Current ( A ) ---> ')
%ylabel(' Number of electrons ---> ')
grid on
```

% Fig.E.1.4

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;q=1.602e-19;I0=q*q/hbar;

%Parameters
U0=0.025;kT=0.025;mu=0;ep=0.2;N0=0;
g1=0.005;g2=0.005;g=g1+g2;
alphag=1;alphad=0.5;

%Energy grid
NE=501;E=linspace(-1,1,NE);dE=E(2)-E(1);
```

```
g1=0.005*(E+abs(E))./(E+E+1e-6);% zero for negative E
g2=0.005*ones(1,NE);
g=g1+g2;

%Bias
IV=101;VV=linspace(-.6,.6,IV);
for iV=1:IV
    Vg=0;Vd=VV(iV);
    %Vd=0;Vg=VV(iV);
        mu1=mu;mu2=mu1-Vd;UL=-(alphag*Vg)-(alphad*Vd);

U=0;%Self-consistent field
dU=1;
while dU>1e-6
    f1=1./(1+exp((E-mu1)./kT));
        f2=1./(1+exp((E-mu2)./kT));
        D=(g./(2*pi))./(((E-ep-UL-U).^2)+((g./2).^2));
            D=D./(dE*sum(D));
    N(iV)=dE*2*sum(D.*((f1.*g1./g)+(f2.*g2./g)));
        Unew=U0*(N(iV)-N0);dU=abs(U-Unew);
            U=U+0.1*(Unew-U);
end
I(iV)=dE*2*I0*(sum(D.*(f1-f2).*g1.*g2./g));
end

hold on
%h=plot(VV,N/2,'b');%Part (a)
h=plot(VV,I,'b');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[25])
xlabel(' Voltage (V) --->')
ylabel(' Current (A) ---> ')
%ylabel(' Number of electrons ---> ')
grid on
```

Chapter 2

% Fig.2.3.2a, b

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;m=9.110e-31;epsil=8.854e-12;q=1.602e-19;

%Lattice
Np=100;a=1e-10;X=a*[1:1:Np];t0=(hbar^2)/(2*m*(a^2))/q;L=a*(Np+1);
T=(2*t0*diag(ones(1,Np)))-(t0*diag(ones(1,Np-1),1))-(t0*diag(ones(1,Np-1),-1));

[V,D]=eig(T);D=diag(D);[Enum,ind]=sort(D);

E1=D(ind(1));psi1=abs(V(:,ind(1)));P1=psi1.*conj(psi1);
E2=D(ind(25));psi2=abs(V(:,ind(25)));P2=psi2.*conj(psi2);
```

```
%analytical eigenvalues
Ean=(((hbar*pi)^2)/(2*m*(L^2))/q)*[1:Np].*[1:Np];

hold on
%h=plot(Enum,'bx');% Part (a)
%h=plot(Ean,'b');% Part (a)
h=plot(P1,'b');% Part (b)
h1=plot(P2,'b');% Part (b)
set(h,'linewidth',[3.0])
set(h1,'linewidth',[1.0])
set(gca,'Fontsize',[25])

%xlabel(' Eigenvalue Number , alpha --->');% Part (a)
%ylabel(' E (eV) ---> ');% Part (a)
xlabel(' Lattice site # --->');% Part (b)
ylabel(' Probability ---> ');% Part (b)
grid on
```

% Fig.2.3.5

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;m=9.110e-31;epsil=8.854e-12;q=1.602e-19;

%Lattice
Np=100;a=1e-10;X=a*[1:1:Np];t0=(hbar^2)/(2*m*(a^2))/q;L=a*(Np+1);
T=(2*t0*diag(ones(1,Np)))-(t0*diag(ones(1,Np-1),1))-(t0*diag(ones(1,Np-1),-1));
T(1,Np)=-t0;T(Np,1)=-t0;

[V,D]=eig(T);D=diag(D);[Enum,ind]=sort(D);

E1=D(ind(1));psi1=abs(V(:,ind(1)));P1=psi1.*conj(psi1);
E2=D(ind(50));psi2=abs(V(:,ind(50)));P2=psi2.*conj(psi2);

%analytical eigenvalues
Ean=(((hbar*pi)^2)/(2*m*(L^2))/q)*[1:Np].*[1:Np];

hold on
h=plot(Enum,'bx');
set(h,'linewidth',[3.0])
set(gca,'Fontsize',[25])
xlabel(' Eigenvalue Number, alpha --->');
ylabel(' E (eV) ---> ');
grid on
```

% Fig.2.3.6, 2.3.7

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;m=9.110e-31;epsil=8.854e-12;q=1.602e-19;
a0=4*pi*epsil*hbar*hbar/(m*q*q),E0=q/(8*pi*epsil*a0)
```

```
%Lattice
Np=100;a=(5e-10*2/Np);% *1 for Fig.1.3.6 and *2 for Fig.1.3.7
R=a*[1:1:Np];t0=(hbar^2)/(2*m*(a^2))/q;

%Quantum numbers
n=1;l=0;% for 1s, n=1 and for 2s, n=2

%Hamiltonian,H = Kinetic,K + Potential,U
K=(2*t0*diag(ones(1,Np)))-(t0*diag(ones(1,Np-1),1))-(t0*diag(ones(1,Np-1),-1));
U=((-q/(4*pi*epsil)./R)+(l*(l+1)*hbar*hbar/(2*m*q))./(R.*R));U=diag(U);
[V,D]=eig(K+U);D=diag(D);[DD,ind]=sort(D);
E=D(ind(n-l));psi=V(:,ind(n-l));
P=psi.*conj(psi);[-E0/(n^2) E]

%analytical solutions
P1s=(4*a/(a0^3))*R.*R.*exp(-2*R./a0);
P2s=(4*a/(2*4*4*(a0^3)))*R.*R.*((2-(R./a0)).^2).*exp(-2*R./(2*a0));
P3s=(4*a/(3*81*81*(a0^3)))*R.*R.*((27-(18*R./a0)+(2*(R./a0).^2)).^2).*exp(-2*R./(3*a0));
P2p=(4*a/(3*32*(a0^3)))*R.*R.*((R./a0).^2).*exp(-2*R./(2*a0));
P3p=(8*a/(3*81*81*(a0^3)))*R.*R.*((6-(R./a0)).^2).*((R./a0).^2).*exp(-2*R./(3*a0));

hold on
h=plot(R,P,'b');
h=plot(R,P1s,'bx');% use P1s for '1s' and P2s for '2s'
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[25])
xlabel(' x (m ) --->');
ylabel(' Probability ---> ');
grid on
```

Chapter 3

% Fig.3.1.4

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;m=9.110e-31;epsil=8.854e-12;q=1.602e-19;
%Lattice
Np=200;a=(10e-10/Np);R=a*[1:1:Np];t0=(hbar^2)/(2*m*(a^2))/q;

%Hamiltonian,H = Kinetic,T + Potential,U + Uscf
T=(2*t0*diag(ones(1,Np)))-(t0*diag(ones(1,Np-1),1))-(t0*diag(ones(1,Np-1),-1));
UN=(-q*2/(4*pi*epsil))./R;% Z=2 for Helium

Uscf=zeros(1,Np);change=1;
while change>0.01
    [V,D]=eig(T+diag(UN+Uscf));D=diag(D);[DD,ind]=sort(D);
    E=D(ind(1));psi=V(:,ind(1));P=psi.*conj(psi);P=P';
        Unew=(q/(4*pi*epsil))*((sum(P./R)-cumsum(P./R))+(cumsum(P)./R));
        change=sum(abs(Unew-Uscf))/Np,Uscf=Unew;
end
```

```
%analytical solutions for 1s hydrogen
a0=4*pi*epsil*hbar*hbar/(m*q*q);
P0=(4*a/(a0^3))*R.*R.*exp(-2*R./a0);

hold on
%h=plot(R,UN,'b');% Part (a)
%h=plot(R,Uscf,'b');% Part(a)
h=plot(R,P,'b');% Part (b)
h=plot(R,P0,'bx');% Part (b)
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[25])
xlabel(' R ( m ) --->');
%ylabel(' U ( eV ) ---> ');% Part (a)
%axis([0 1e-9 -100 20]);% Part (a)
ylabel(' Probability ---> ');% Part (b)
axis([0 1e-9 0 0.1]);% Part (b)
grid on
```

% Fig.3.1.5

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;m=9.110e-31;epsil=8.854e-12;q=1.602e-19;

%Lattice
Np=200;a=(10e-10/Np);R=a*[1:1:Np];t0=(hbar^2)/(2*m*(a^2))/q;

%Hamiltonian,H = Kinetic,T + Potential,U + Ul + Uscf
T=(2*t0*diag(ones(1,Np)))-(t0*diag(ones(1,Np-1),1))-(t0*diag(ones(1,Np-1),-1));
UN=(-q*14/(4*pi*epsil))./R;% Z=14 for silicon
l=1;Ul=(l*(l+1)*hbar*hbar/(2*m*q))./(R.*R);

Uscf=zeros(1,Np);change=1;
while change>0.1
    [V,D]=eig(T+diag(UN+Uscf));D=diag(D);[DD,ind]=sort(D);
    E1s=D(ind(1));psi=V(:,ind(1));P1s=psi.*conj(psi);P1s=P1s';
    E2s=D(ind(2));psi=V(:,ind(2));P2s=psi.*conj(psi);P2s=P2s';
    E3s=D(ind(3));psi=V(:,ind(3));P3s=psi.*conj(psi);P3s=P3s';

    [V,D]=eig(T+diag(UN+Ul+Uscf));D=diag(D);[DD,ind]=sort(D);
    E2p=D(ind(1));psi=V(:,ind(1));P2p=psi.*conj(psi);P2p=P2p';
    E3p=D(ind(2));psi=V(:,ind(2));P3p=psi.*conj(psi);P3p=P3p';
    n0=(2*(P1s+P2s+P3s))+(6*P2p)+(2*P3p);

    n=n0*(13/14);
    Unew=(q/(4*pi*epsil))*((sum(n./R)-cumsum(n./R))+(cumsum(n)./R));
    %Uex=(-q/(4*pi*epsil))*((n./(4*pi*a*R.*R)).^(1/3));%Unew=Unew+Uex;
    change=sum(abs(Unew-Uscf))/Np,Uscf=Unew;
end

[E1s E2s E2p E3s E3p]
```

```
%analytical solution for 1s hydrogen
a0=4*pi*epsil*hbar*hbar/(m*q*q);
P0=(4*a/(a0^3))*R.*R.*exp(-2*R./a0);

hold on
h=plot(R,P1s,'b');
h=plot(R,P0,'bx');
h=plot(R,P3p,'bo');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[25])
xlabel(' R ( m ) --->');
ylabel(' Probability ---> ');
axis([0 5e-10 0 0.08]);
grid on
```

% Fig.3.3.4

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;m=9.110e-31;epsil=8.854e-12;q=1.602e-19;
a0=4*pi*epsil*hbar*hbar/(m*q*q);E0=q/(8*pi*epsil*a0);

R0=.05*[1:200];
a=(-2*E0)*(1-(exp(-2*R0).*(1+R0)))./R0;
b=(-2*E0)*exp(-R0).*(1+R0);
s=(1+R0+((R0.^2)/3)).*exp(-R0);
Uee=(2*E0)./sqrt(1+(R0.^2));UNN=(2*E0)./R0;

EB0=(a+b)./(1+s);R=a0*R0;

hold on
h=plot(R,EB0,'b--');
h=plot(R,Uee,'bx');
h=plot(R,UNN,'b');
h=plot(R,(2*EB0)+UNN+Uee,'b+');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[25])
grid on
xlabel(' R ( m ) --->')
ylabel(' Energy (eV) ---> ')
axis([0 4e-10 -25 25])
```

% Fig.3.4.2

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;q=1.602e-19;I0=q*q/hbar;

%Parameters
U0=0.5;% U0 is 0.25 for part(a), 0.1 for part (b)
```

```
kT=0.025;mu=0;ep=0.2;
g1=0.005;g2=0.005;g=g1+g2;
alphag=1;alphad=0.5;

%Bias
IV=101;VV=linspace(0,1,IV);
for iV=1:IV
    Vd=0;Vg=VV(iV);
        mu1=mu;mu2=mu1-Vd;UL=-(alphag*Vg)-(alphad*Vd);
f1=1/(1+exp((ep+UL-mu1)/kT));f2=1/(1+exp((ep+UL-mu2)/kT));
f1U=1/(1+exp((ep+UL+U0-mu1)/kT));f2U=1/(1+exp((ep+UL+U0-mu2)/kT));

P1=((g1*f1)+(g2*f2))/(1e-6+(g1*(1-f1))+(g2*(1-f2)));
P2=P1*((g1*f1U)+(g2*f2U))/(1e-6+(g1*(1-f1U))+(g2*(1-f2U)));
P0=1/(1+P1+P1+P2);P1=P1*P0;P2=P2*P0;
p0(iV)=P0;p1(iV)=P1;p2(iV)=P2;
end

hold on
h=plot(VV,p0,'bo');
h=plot(VV,p1,'b');
h=plot(VV,p2,'bx');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[25])
grid on
xlabel(' Gate voltage, VG ( volts ) --->')
ylabel(' Current ( Amperes ) ---> ')
axis([0 1 0 1])
```

% Fig.3.4.3

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;q=1.602e-19;I0=q*q/hbar;

%Parameters
U0=0.1;% U0 is 0.25 for part(a), 0.025 for part (b)
kT=0.025;mu=0;ep=0.2;
g1=0.005;g2=0.005;g=g1+g2;
alphag=1;alphad=0.5;

%Bias
IV=101;VV=linspace(0,1.5,IV);
for iV=1:IV
    Vg=0;Vd=VV(iV);
    %Vd=0;Vg=VV(iV);
        mu1=mu;mu2=mu1-Vd;UL=-(alphag*Vg)-(alphad*Vd);

%Multielectron method
f1=1/(1+exp((ep+UL (-U0/2)-mu1)/kT));f2=1/(1+exp((ep+UL(-U0/2)-mu2)/kT));
f1U=1/(1+exp((ep+UL+(U0/2)-mu1)/kT));f2U=1/(1+exp((ep+UL+(U0/2)-mu2)/kT));
```

```
P1=((g1*f1)+(g2*f2))/(1e-6+(g1*(1-f1))+(g2*(1-f2)));
P2=P1*((g1*f1U)+(g2*f2U))/(1e-6+(g1*(1-f1U))+(g2*(1-f2U)));
P0=1/(1+P1+P1+P2);P1=P1*P0;P2=P2*P0;

I1(iV)=2*I0*((P0*g1*f1)-(P1*g1*(1-f1))+(P1*g1*f1U)-(P2*g1*(1-f1U)));
I2(iV)=2*I0*((P0*g2*f2)-(P1*g2*(1-f2))+(P1*g2*f2U)-(P2*g2*(1-f2U)));
end

%RSCF method (same as Fig.1.4.6 with added factor of two)
%Energy grid
NE=501;E=linspace(-1,1,NE);dE=E(2)-E(1);
D=(g/(2*pi))./((E.^2)+((g/2)^2));% Lorentzian Density of states per eV
D=D./(dE*sum(D));%Normalizing to one

%Bias
for iV=1:IV
    Vg=0;Vd=VV(iV);
    %Vd=0;Vg=VV(iV);
        mu1=mu;mu2=mu1-Vd;UL=-(alphag*Vg)-(alphad*Vd);

U=0;%Self-consistent field
dU=1;
while dU>1e-6
    F1=1./(1+exp((E+ep+UL+U-mu1)./kT));
        F2=1./(1+exp((E+ep+UL+U-mu2)./kT));
    N(iV)=dE*2*sum(D.*((F1.*g1/g)+(F2.*g2/g)));
        Unew=U0*N(iV);
        dU=abs(U-Unew);U=U+0.1*(Unew-U);
end
I(iV)=dE*2*I0*(sum(D.*(F1-F2)))*(g1*g2/g);
end

hold on
h=plot(VV,I1,'b');
h=plot(VV,I,'b--');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[25])
grid on
xlabel(' Drain Voltage, VD ( volts ) --->')
ylabel(' Current ( Amperes ) ---> ')
axis([0 1.5 0 1.4e-6])

%E.3.5c: Unrestricted scf
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;q=1.602e-19;I0=q*q/hbar;

%Parameters
U0=0.25;kT=0.025;mu=0;ep=0.2;
g1=0.005;g2=0.005;g=g1+g2;
alphag=1;alphad=0.5;
```

```
%Energy grid
NE=501;E=linspace(-1,1,NE);dE=E(2)-E(1);
D=(g/(2*pi))./((E.^2)+((g/2)^2));% Lorentzian Density of states per eV
D=D./(dE*sum(D));%Normalizing to one

%Bias
IV=101;VV=linspace(0,1,IV);
for iV=1:IV
    Vg=0;Vd=VV(iV);
    %Vd=0;Vg=VV(iV);
        mu1=mu;mu2=mu1-Vd;UL=-(alphag*Vg)-(alphad*Vd);

Uup=0;Udn=0.1;%Unrestricted self-consistent field
dU=1;while dU>.001
    f1up=1./(1+exp((E+ep+UL+Uup-mu1)./kT));
        f2up=1./(1+exp((E+ep+UL+Uup-mu2)./kT));
            Nup(iV)=dE*sum(D.*((f1up.*g1)+(f2up.*g2))./(g1+g2));
    f1dn=1./(1+exp((E+ep+UL+Udn-mu1)./kT));
        f2dn=1./(1+exp((E+ep+UL+Udn-mu2)./kT));
            Ndn(iV)=dE*sum(D.*((f1dn.*g1)+(f2dn.*g2))./(g1+g2));
            Udnnew=2*U0*(Nup(iV)-0.5);Udn=Udn+0.1*(Udnnew-Udn);
            Uupnew=2*U0*(Ndn(iV)-0.5);Uup=Uup+0.1*(Uupnew-Uup);
                dU=abs(Uup-Uupnew)+abs(Udn-Udnnew);
end
Iup(iV)=dE*I0*sum(D.*(f1up-f2up))*(g1*g2/g);
Idn(iV)=dE*I0*sum(D.*(f1dn-f2dn))*(g1*g2/g);
end

hold on
%h=plot(VV,Nup,'bo');%Part (b)
%h=plot(VV,Ndn,'bx');%Part (b)
h=plot(VV,Iup+Idn,'b');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[25])
xlabel(' Voltage (V) --->')
ylabel(' Current (A) ---> ')
%ylabel(' Number of electrons ---> ');%Part (b)
grid on
```

Chapter 4

% Fig.4.1.4

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;m=9.110e-31;epsil=8.854e-12;q=1.602e-19;
a0=4*pi*epsil*hbar*hbar/(m*q*q);E0=q/(8*pi*epsil*a0);
```

```
%Basis
L=.074e-9/a0;s=exp(-L)*(1+L+((L^2)/3));
r=linspace(-2e-10,+2e-10,101);r0=r/a0;
psi=sqrt(1/(pi*(a0^3)))*(exp(-abs(r0-(L/2)))+exp(-abs(r0+(L/2))));
n=2*psi.*conj(psi)./(2*(1+s));

a=-2*E0*(1-((1+L)*exp(-2*L)))/L;
b=-2*E0*(1+L)*exp(-L);
EB0=-E0+((a+b)/(1+s));
[a b s EB0]

hold on
h=plot(r,n,'b');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[25])
grid on
xlabel(' R ( m ) --->')
ylabel(' Electron density ( /m^3 ) ---> ')
axis([-2e-10 2e-10 0 2e30])
```

% Fig.4.3.1

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;m=9.110e-31;q=1.602e-19;mu=0.25;
kT=0.025;% 0.025 for Part (c),(e) and 0.0025 for Part (d),(f)

%Lattice
Np=100;a=2e-10;X=a*[1:1:Np];t0=(hbar^2)/(2*m*(a^2))/q;U=linspace(0,0,Np);
T=(2*t0*diag(ones(1,Np)))-(t0*diag(ones(1,Np-1),1))-(t0*diag(ones(1,Np-1),-1));
T(1,Np)=-t0;T(Np,1)=-t0;%Periodic boundary conditions for Parts (d), (f)
U(Np/2)=U(Np/2)+10;%Impurity potential with Parts (d), (f)

[V,D]=eig(T+diag(U));E=sort(diag(D)');
D=diag(D)-mu;
rho=1./(1+exp(D./kT));rho=V*diag(rho)*V';rho=diag(rho)/a;

hold on
grid on
%h=plot(E,'b');h=plot(mu*ones(Np/2,1),'b');% Part (b)
h=plot(X,rho,'b');% Part (c)-(f)
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[25])
grid on
%xlabel(' Eigenvalues number --->');% Part (b)
%ylabel(' Energy ( eV ) ---> ');% Part (b)
xlabel(' x ( m ) --->');% Part (c)-(f)
ylabel(' Electron density ( /m^3 ) ---> ');% Part (c)-(f)
```

```
%axis([0 100 0 4]);% Part (b)
axis([0 2e-8 0 1e9]);% Part (c)-(f)
```

% Fig.4.4.1, 4.4.2

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;m=9.110e-31;epsil=8.854e-12;q=1.602e-19;
a0=4*pi*epsil*hbar*hbar/(m*q*q);E0=q/(8*pi*epsil*a0);

F=linspace(0,1e9,11);A=(a0*128*sqrt(2)/243)*F;B=(-3*a0)*F;
for kF=1:11
M=[-E0 0 A(kF);0 -E0/4 B(kF);A(kF) B(kF) -E0/4];
[V,D]=eig(M);D=diag(D);[DD,ind]=sort(D);
E1(kF)=D(ind(1));E2(kF)=D(ind(2));E3(kF)=D(ind(3));
end

%perturbation theory results
E1s=-E0-((A.^2)/(3*E0/4));
E2s=-(E0/4)+B;
E2p=-(E0/4)-B;

hold on
%h=plot(F,E1,'b');% Fig.3.4.1
%h=plot(F,E1s,'bx');% Fig.3.4.1
h=plot(F,E2,'b');% Fig.3.4.2
h-plot(F,E3,'b');% Fig.3.4.2
h=plot(F,E2s,'bx');% Fig.3.4.2
h=plot(F,E2p,'bo');% Fig.3.4.2
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[25])
grid on
xlabel(' Field ( V/m ) --->');
ylabel(' Energy ( eV ) ---> ');
%axis([0 2e-8 0 1e9]);
```

Chapter 5

% Fig.5.1.5

```
clear all

k=linspace(-1,1,21);a=2;b=1;
E1=sqrt((a^2)+(b^2)+(2*a*b.*cos(pi*k)));

hold on
h=plot(k,E1,'b');
h=plot(k,-E1,'b');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[25])
xlabel('k (in units of pi/a)--->')
```

```
ylabel('Energy (eV) ---> ')
grid on
```

% Fig.5.3.2

```
clear all

Esa=-8.3431;Epa=1.0414;Esc=-2.6569;Epc=3.6686;Esea=8.5914;Esec=6.7386;
Vss=-6.4513;Vxx=1.9546;Vxy=5.0779;Vsapc=4.4800;Vpasc=5.7839;Vseapc=4.8422;
Vpasec=4.8077;

%Either of the following choices for d1,d2,d3 and d4 should give the same result.
d1=[1 1 1]/4;d2=[1 -1 -1]/4;d3=[-1 1 -1]/4;d4=[-1 -1 1]/4;
d1=[0 0 0]/2;d2=[0 -1 -1]/2;d3=[-1 0 -1]/2;d4=[-1 -1 0]/2;

l=1;m=1;n=1;kmax=pi;Nt=21;%L-direction
%l=1;m=0;n=0;kmax=2*pi;Nt=21;%X-direction

for Nk=1:Nt
k=[l m n]*kmax*(Nk-1)/(Nt-1);
      p1=exp(i*sum(k.*d1));p2=exp(i*sum(k.*d2));
      p3=exp(i*sum(k.*d3));p4=exp(i*sum(k.*d4));
            g0=(p1+p2+p3+p4)/4;g1=(p1+p2-p3-p4)/4;
            g2=(p1-p2+p3-p4)/4;g3=(p1-p2-p3+p4)/4;

h=[Esa/2 Vss*g0 0 0 0 Vsapc*g1 Vsapc*g2 Vsapc*g3 0 0;
    0    Esc/2    -Vpasc*conj(g1)    -Vpasc*conj(g2)    -Vpasc*conj(g3)     0 0 0 0 0;
    0    0        Epa/2  0           0        Vxx*g0     Vxy*g3 Vxy*g2   0 -Vpasec*g1;
    0    0        0      Epa/2       0        Vxy*g3     Vxx*g0 Vxy*g1 0 -Vpasec*g2;
    0    0        0      0           Epa/2    Vxy*g2     Vxy*g1 Vxx*g0 0 -Vpasec*g3;
    0    0        0      0           0        Epc/2      0      0      Vseapc*(g1)      0;
    0    0        0      0           0        0          Epc/2  0      Vseapc*(g2)      0;
    0    0        0      0           0        0          0      Epc/2  Vseapc*(g3)      0;
    0    0        0      0           0        0          0      0      Esea/2    0;
    0    0        0      0           0        0          0      0      0         Esec/2];
H=h+h';
[V,D]=eig(H);
      eigst = sum(D);
      E(Nk,:) = sort(real(eigst));
            X(Nk)=-(Nk-1)/(Nt-1);%L-direction
            X1(Nk)=(Nk-1)/(Nt-1);%X-direction
end

hold on
h=plot(X,E,'b');
%h=plot(X1,E,'b');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[25])
xlabel('k (as fraction of maximum value)--->')
ylabel('Energy (eV) ---> ')
grid on
```

```
%Note: X-axis from 0 to +1 represents the -X direction
%while the section from 0 to -1 represents the -L direction
```

```
% Fig.5.4.1a

clear all

soa=.3787/3;soc=.0129/3;Esa=-8.3431;Epa=1.0414;Esc=-2.6569;Epc=3.6686;Esea=8.5914;
Esec=6.7386;Vss=-6.4513;Vxx=1.9546;Vxy=5.0779;Vsapc=4.4800;
Vpasc=5.7839;Vseapc=4.8422;Vpasec=4.8077;
d1=[1 1 1]/4;d2=[1 -1 -1]/4;d3=[-1 1 -1]/4;d4=[-1 -1 1]/4;
d1=[0 0 0]/2;d2=[0 -1 -1]/2;d3=[-1 0 -1]/2;d4=[-1 -1 0]/2;

l=1;m=1;n=1;kmax=pi;Nt=101;%L-direction
l=1;m=0;n=0;kmax=2*pi;Nt=101;%X-direction

for Nk=1:Nt
k=[l m n]*kmax*(Nk-1)/(Nt-1);
      p1=exp(i*sum(k.*d1));p2=exp(i*sum(k.*d2));
      p3=exp(i*sum(k.*d3));p4=exp(i*sum(k.*d4));
            g0=(p1+p2+p3+p4)/4;g1=(p1+p2-p3-p4)/4;
            g2=(p1-p2+p3-p4)/4;g3=(p1-p2-p3+p4)/4;

h=[Esa/2 Vss*g0 0 0 0 Vsapc*g1 Vsapc*g2 Vsapc*g3 0 0;
    0   Esc/2   -Vpasc*conj(g1)   -Vpasc*conj(g2)   -Vpasc*conj(g3)    0 0 0 0 0;
    0   0       Epa/2  0          0       Vxx*g0     Vxy*g3 Vxy*g2   0 -Vpasec*g1;
    0   0       0      Epa/2      0       Vxy*g3     Vxx*g0 Vxy*g1 0 -Vpasec*g2;
    0   0       0      0          Epa/2   Vxy*g2     Vxy*g1 Vxx*g0 0 -Vpasec*g3;
    0   0       0      0          0       Epc/2      0      0        Vseapc*(g1)      0;
    0   0       0      0          0       0          Epc/2  0        Vseapc*(g2)      0;
    0   0       0      0          0       0          0      Epc/2    Vseapc*(g3)      0;
    0   0       0      0          0       0          0      0        Esea/2    0;
    0   0       0      0          0       0          0      0        0         Esec/2];
H=[h+h' zeros(10);
      zeros(10)    h+h'];

hso=zeros(20);
hso(3,4)=-i*soa;hso(3,15)=soa;
hso(4,15)=-i*soa;
hso(5,13)=-soa;hso(5,14)=i*soa;
hso(6,7)=-i*soc;hso(6,18)=soc;
hso(7,18)=-i*soc;
hso(8,16)=-soc;hso(8,17)=i*soc;
hso(13,14)=i*soa;
hso(16,17)=i*soc;
Hso=hso+hso';

[V,D]=eig(H+Hso);
      eigst = sum(D);
      E(Nk,:) = sort(real(eigst));
```

```
            X(Nk)=-(Nk-1)/(Nt-1);%L-direction
            X1(Nk)=(Nk-1)/(Nt-1);%X-direction
end

hold on
%h=plot(X,E,'b');
h=plot(X1,E,'b');
axis([-1 1 -3 3])
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[25])
xlabel('k (as fraction of maximum value)--->')
ylabel('Energy (eV) ---> ')
grid on
```

Chapter 6

```
% Fig.6.1.2

clear all

z=zeros(5);Z=zeros(10);
%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;q=1.602e-19;a=2.45e-10*4/sqrt(3);m=9.110e-31;
d1=[1 1 1]/4;d2=[1 -1 -1]/4;d3=[-1 1 -1]/4;d4=[-1 -1 1]/4;

%sp3s* model parameters
soa=.3787/3;soc=.0129/3;
Esa=-8.3431;Epa=1.0414;Esc=-2.6569;Epc=3.6686;Esea=8.5914;Esec=6.7386;
Vss=-6.4513;Vpasc=-5.7839;Vpasec=-4.8077;
Vsapc=4.4800;Vseapc=4.8422;Vxx=1.9546;Vxy=5.0779;

%Conduction band effective mass model parameters
Ec=1.55;meff=.12*m;

Nt=101;kk=1*linspace(0,1,Nt);
l=0.5;m=0.5;n=0.5;%L-direction
%l=1;m=0;n=0;%X-direction

for Nk=1:Nt
k=2*pi*kk(Nk)*[l m n];

%sp3s* model
    p1=exp(i*sum(k.*d1));p2=exp(i*sum(k.*d2));
    p3=exp(i*sum(k.*d3));p4=exp(i*sum(k.*d4));
        g0=(p1+p2+p3+p4)/4;g1=(p1+p2-p3-p4)/4;
        g2=(p1-p2+p3-p4)/4;g3=(p1-p2-p3+p4)/4;

a1=diag([Esa Epa Epa Epa Esea]);A1=[a1 z;z a1];
a2=diag([Esc Epc Epc Epc Esec]);A2=[a2 z;z a2];
b=[Vss*g0 Vsapc*g1 Vsapc*g2 Vsapc*g3 0;
    Vpasc*g1    Vxx*g0 Vxy*g3 Vxy*g2 Vpasec*g1;
    Vpasc*g2 Vxy*g3 Vxx*g0 Vxy*g1 Vpasec*g2;
```

```
    Vpasc*g3 Vxy*g2 Vxy*g1 Vxx*g0 Vpasec*g3;
    0 Vseapc*conj(g1) Vseapc*conj(g2) Vseapc*conj(g3) 0];B=[b z;z b];
    h=[a1 b;b' a2];H=[A1 B;B' A2];

aso=soa*[0 0 0 0 0 0 0 0 0 0;
            0 0 -i 0 0 0 0 0 1 0;
            0 i 0 0 0 0 0 0 -i 0;
            0 0 0 0 0 0 -1 i 0 0;
            0 0 0 0 0 0 0 0 0 0;
            0 0 0 0 0 0 0 0 0 0;
            0 0 0 -1 0 0 0 i 0 0;
            0 0 0 -i 0 0 -i 0 0 0;
            0 1 i 0 0 0 0 0 0 0;
            0 0 0 0 0 0 0 0 0 0];
    cso=soc*[0 0 0 0 0 0 0 0 0 0;
            0 0 -i 0 0 0 0 0 1 0;
            0 i 0 0 0 0 0 0 -i 0;
            0 0 0 0 0 0 -1 i 0 0;
            0 0 0 0 0 0 0 0 0 0;
            0 0 0 0 0 0 0 0 0 0;
            0 0 0 -1 0 0 0 i 0 0;
            0 0 0 -i 0 0 -i 0 0 0;
            0 1 i 0 0 0 0 0 0 0;
            0 0 0 0 0 0 0 0 0 0];H=H+[aso Z;Z cso];

[V,D]=eig(H);
    eiglst = sum(D);
    E(Nk,:) = sort(real(eiglst));

%Conduction band effective mass model
Em(Nk)=Ec+((hbar^2)*sum(k.*k)/(2*meff*q*(a^2)));
end

kk=-kk;%L-direction

hold on
h1=plot(kk,E, 'b');
h2=plot(kk,Em,'b--');
axis([-1 1 -3 3])
set(h1,'linewidth',[1.0])
set(h2,'linewidth',[2.0])
set(gca,'Fontsize',[24])
xlabel(' ka (fraction of maximum value ---> ')
ylabel(' Energy ( eV ) ---> ')
grid on
```

% Fig.6.1.7

```
clear all

t=3;m=65;%66 for (a), 65 for (b)
D=2*m*0.14*sqrt(3)/(2*pi);
```

```
Eg=2*t*0.14/D;nu=round(2*m/3)+0;% +1 is used for higher mode
kyb=2*pi*nu/(2*m);
kxa=0.05*linspace(-pi,pi,101);

E1=(3*t/2)*sqrt(((kxa*2/3).^2)+(((abs(kyb)-(2*pi/3))*2/sqrt(3)).^2));%a0=b*2/sqrt(3)=a*2/3;
E2=t*sqrt(1+(4*cos(kyb).*cos(kxa))+(4*cos(kyb).^2));

k=kxa./pi;[D Eg nu min(E1)]

hold on
h=plot(k,E1, 'b');
h=plot(k,-E1, 'b');
axis([-0.05 0.05 -0.6 0.6])
set(h,'linewidth',[1.0])
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
xlabel(' kxa/pi (fraction of maximum value ---> ')
ylabel(' Energy ( eV ) ---> ')
grid on
```

% Fig.6.1.9

```
clear all

t=3;kxa=0;
kyb=linspace(-pi,pi,101);
E1=(3*t/2)*sqrt(((kxa*2/3).^2)+(((abs(kyb)-(2*pi/3))*2/sqrt(3)).^2));%a0=b*2/sqrt(3)=a*2/3;
E2=t*sqrt(1+(4*cos(kyb).*cos(kxa))+(4*cos(kyb).^2));

k=kyb./pi;

hold on
h=plot(k,E1,'b');
h=plot(k,-E1,'b');
h=plot(k,E2,'bx');
h=plot(k,-E2,'bx');
axis([-1 1 -15 15])
set(h,'linewidth',[1.0])
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
xlabel(' kyb/pi ---> ')
ylabel(' Energy ( eV ) ---> ')
grid on
```

% Fig.6.2.1

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;m=9.110e-31;q=1.602e-19;L=1e-9;
D2=zeros(1,101);
```

```
Lz=20e-9;%5e-9 for (a),20e-9 for (b)
E0=(hbar^2)*(pi^2)/(2*q*m*Lz^2);
for p=1:25
E=linspace(-0.1,0.25,101);thet=(E+abs(E))./(2*E);
EE=E-(p*p*E0);theta=(EE+abs(EE))./(2*EE);
D1=(L)*q*m*thet.*real((2*m*E*q).^(-0.5))./(pi*hbar);
D2=D2+((L^2)*q*m*theta./(2*pi*hbar*hbar));
D3=(L^3)*q*m*thet.*real((2*m*E*q).^0.5)./(2*pi*pi*hbar*hbar*hbar);
end

hold on
h=plot(D2,E,'b');
h=plot(D3.*Lz/L,E,'b');
%axis([0 10 -0.1 0.25]);%Part (a)
axis([0 40 -0.1 0.25]);%Part (b)
set(h,'linewidth',[1.0])
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
xlabel(' D(E) (per eV per nm^2) ---> ')
ylabel(' Energy ( eV ) ---> ')
grid on
```

% Fig.6.2.2

```
clear all

t=3;m=800;% Use 200 and 800 for two plots
a0=0.14;D=2*m*a0*sqrt(3)/(2*pi);Eg=2*t*0.14/D;c=pi*D;L=1;D
nu0=round(2*m/3);a=3*a0/2;

E=linspace(0,0.25,101);
DG=(2*c*L/(2*pi*a*a*t*t))*E;

DN=zeros(1,101);
for nu=nu0-100:nu0+100
Ek=((t*2*pi/sqrt(3))*((3*nu/(2*m))-1))+(i*1e-12);
    DN=DN+((2*L/(pi*a*t))*abs(real(E./(sqrt((E.^2)-(Ek^2))))));
end

hold on
h1=plot(DG,E,'bx');
h2=plot(DN,E,'b');
hold on
axis([0 50 0 0.25]);
set(h1,'linewidth',[1.0])
set(h2,'linewidth',[2.0])
set(gca,'Fontsize',[24])
xlabel(' D(E) (per eV per nm) ---> ')
ylabel(' Energy ( eV ) ---> ')
grid on
```

% Fig.6.3.3

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;m=9.110e-31;q=1.602e-19;a=5e-10;L=10e-9;

k=0.5*linspace(-1,1,201)/a;
Ek=(hbar^2)*(k.^2)/(2*0.25*m*q);
EE=linspace(0,0.2,201);

%Subband (1,1)
E1=2*(hbar^2)*(pi^2)/(2*0.25*m*q*L^2);
M=((EE-E1)+abs(EE-E1))./(2*abs(EE-E1));

%Subbands (1,2) and (2,1)
E2=5*(hbar^2)*(pi^2)/(2*0.25*m*q*L^2);
M=M+(((EE-E2)+abs(EE-E2))./(abs(EE-E2)));

%Subband (2,2)
E3=8*(hbar^2)*(pi^2)/(2*0.25*m*q*L^2);
M=M+(((EE-E3)+abs(EE-E3))./(2*abs(EE-E3)));

hold on
h=plot(k,E1+Ek,'b');%Part (a)
h=plot(k,E2+Ek,'b');%Part (a)
h=plot(k,E3+Ek,'b');%Part (a)
%h=plot(M,EE,'b');%Part (b)
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
xlabel('k ( / m )');%Part (a)
%xlabel(' M ( E ) ');%Part (b)
ylabel('E - Ec ( eV ) -->');
axis([-1e9 1e9 0 0.3]);%Part (a)
%axis([0 5 0 0.3]);%Part (b)
grid on
```

% Fig.6.3.4

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;m=9.110e-31;q=1.602e-19;a=5e-10;L=10e-9;

k=0.5*linspace(-1,1,201)/a;
Ek=-(hbar^2)*(k.^2)/(2*0.25*m*q);
EE=linspace(0,-0.2,201);

%Subband (1,1)
E1=-2*(hbar^2)*(pi^2)/(2*0.25*m*q*L^2);
M=((E1-EE)+abs(E1-EE))./(2*abs(E1-EE));
```

```
%Subbands (1,2) and (2,1)
E2=-5*(hbar^2)*(pi^2)/(2*0.25*m*q*L^2);
M=M+(((E2-EE)+abs(E2-EE))./(abs(E2-EE)));

%Subband (2,2)
E3=-8*(hbar^2)*(pi^2)/(2*0.25*m*q*L^2);
M=M+(((E3-EE)+abs(E3-EE))./(2*abs(E3-EE)));

hold on
%h=plot(k,E1+Ek,'b');%Part (a)
%h=plot(k,E2+Ek,'b');%Part (a)
%h=plot(k,E3+Ek,'b');%Part (a)
h=plot(M,EE,'b');%Part (b)
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
%xlabel('k ( / m )');%Part (a)
xlabel(' M ( E ) ');%Part (b)
ylabel('E - Ev ( eV ) -->');
%axis([-1e9 1e9 -0.3 0]);%Part (a)
axis([0 5 -0.3 0]);%Part (b)
grid on
```

Chapter 7

% Fig.7.1.5

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;q=1.602e-19;a=3e-10;m=9.110e-31;

%Conduction band parameters
mw=.07*m;ma=.22*m;mb=(.7*mw)+(.3*ma);kk=0*.1*pi;
Ec=0;Eb=(.7*0)+(.3*1.25);

for nk=1:24
Nw=nk+10;Nb=2*Nw;Np=Nb+Nw+Nb;W(nk)=(Nw-1)*a*1e9;
tb=(hbar^2)/(2*mb*(a^2)*q);tw=(hbar^2)/(2*mw*(a^2)*q);
t=[tb*ones(1,Nb) tw*ones(1,Nw-1) tb*ones(1,Nb)];
tt=[0 t]+[t 0];
Ebk=Eb+(tb*(kk^2));Ewk=tw*(kk^2);Ebwk=(Eb/2)+((tb+tw)*(kk^2)/2);
U=Ec+[Ebk*ones(1,Nb) Ebwk Ewk*ones(1,Nw-2) Ebwk Ebk*ones(1,Nb)];
H=-diag(t,1)-diag(t,-1)+diag(tt)+diag(U);
[V,D]=eig(H);D=diag(D);D=(sort(real(D)))';
E1(nk)=D(1);E2(nk)=D(2);

end

hold on
h1=plot(W,E1,'b');
h1=plot(W,E2,'b--');
```

```
set(h1,'linewidth',[2.0])
set(gca,'Fontsize',[24])
xlabel(' W ( nm ) ---> ')
ylabel(' Energy ( eV ) ---> ')
axis([2 10 0 .4])
grid on
```

% Fig.7.1.6

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;q=1.602e-19;a=3e-10;m=9.110e-31;

%Conduction band parameters
mw=.07*m;ma=.22*m;mb=(.7*mw)+(.3*ma);
Nw=24;Nb=2*Nw;Np=Nb+Nw+Nb;W=(Nw-1)*a*1e9
Ec=0;Eb=(.7*0)+(.3*1.25);

for nk=1:26
kk=(nk-1)*a*1e10/500;k(nk)=kk/(a*1e9);
tb=(hbar^2)/(2*mb*(a^2)*q);tw=(hbar^2)/(2*mw*(a^2)*q);
t=[tb*ones(1,Nb) tw*ones(1,Nw-1) tb*ones(1,Nb)];
tt=[0 t]+[t 0];
Ebk=Eb+(tb*(kk^2));Ewk=tw*(kk^2);Ebwk=(Eb/2)+((tb+tw)*(kk^2)/2);
U=Ec+[Ebk*ones(1,Nb) Ebwk Ewk*ones(1,Nw-2) Ebwk Ebk*ones(1,Nb)];
H=-diag(t,1)-diag(t,-1)+diag(tt)+diag(U);
[V,D]=eig(H);D=diag(D);D=(sort(real(D)))';
E1(nk)=D(1);E2(nk)=D(2);
end

E1w=E1(1)+(hbar^2)*(k.^2)./(2*mw*1e-18*q);
E2w=E2(1)+(hbar^2)*(k.^2)./(2*mw*1e-18*q);
E1b=E1(1)+(hbar^2)*(k.^2)./(2*mb*1e-18*q);
E2b=E2(1)+(hbar^2)*(k.^2)./(2*mb*1e-18*q);

hold on
h=plot(k,E1,'b');
h=plot(k,E2,'b');
h=plot(k,E1w,'b:');
h=plot(k,E2w,'b:');
h=plot(k,E1b,'b--');
h=plot(k,E2b,'b--');
set(h,'linewidth',[1.0])
set(gca,'Fontsize',[24])
xlabel(' k ( / nm ) ---> ')
ylabel(' Energy ( eV ) ---> ')
axis([0 .5 0 0.4])
grid on
```

% Fig.7.2.5

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;eps0=8.85E-12;epsr=4;m=.25*9.1e-31;
mu=0;kT=.025;n0=m*kT*q/(2*pi*(hbar^2));n0

%inputs
a=3e-10;t0=(hbar^2)/(2*m*(a^2)*q);e0=q*a/eps0;
Nox=7;Nc=10;%use Nc=10,30 for 3,9nm channel respectively
Np=Nox+Nc+Nox;XX=a*1e9*[1:1:Np];
Ec=[3*ones(Nox,1);0*ones(Nc,1);3*ones(Nox,1)];

%Hamiltonian matrix
T=(2*t0*diag(ones(1,Np)))-(t0*diag(ones(1,Np-1),1))-(t0*diag(ones(1,Np-1),-1));

%dielectric constant matrix
D2=epsr*((2*diag(ones(1,Np)))-(diag(ones(1,Np-1),1))-(diag(ones(1,Np-1),-1)));
iD2=inv(D2);

Vg=.25;Ubdy=-epsr*[Vg;zeros(Np-2,1);Vg];
%Ubdy=-epsr*[0;zeros(Np-2,1);Vg];;%for asymmetric bias
U0=iD2*Ubdy;

%self-consistent calculation
    U1=1e-6*ones(Np,1);UU=U1;change=1;
    while change>1e-3
        U1=U1+(0.1*(UU-U1));
        [P,D]=eig(T+diag(Ec)+diag(U1));D=diag(D);
        rho=log(1+exp((mu-D)./kT));rho=P*diag(rho)*P';
        n=2*n0*diag(rho);
            for kp=1:Np
                ncl(kp)=a*2*(n0^1.5)*Fhalf((mu-Ec(kp)-U1(kp))/kT);
            end
            %n=ncl';%use for semiclassical calculation
            UU=U0+(iD2*e0*n);
            change=max(max((abs(UU-U1))));
        U=Ec+U1;%self-consistent band profile
end

%electron density in channel per cm2
    ns=1e-4*sum(sum(n.*[zeros(Nox,1);ones(Nc,1);zeros(Nox,1)]));Vg,ns
        nn=1e-6*n./a;%electron density per cm3
        Fn=mu*ones(Nc+Nox+Nox,1);

hold on
h=plot(XX,nn,'g');
%h=plot(XX,Ec,'g--');
%h=plot(XX,Ec+U1,'g');
%h=plot(XX,Fn,'g:');
set(h,'linewidth',[2.0])
```

```
set(gca,'Fontsize',[24])
xlabel(' z (nm) ---> ')
%ylabel(' E (eV) ---> ')
ylabel(' n (/cm3) --->')
%axis([0 8 -.5 3])
axis([0 8 0 15e18])
grid on
```

% Fig.7.3.1

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;eps0=8.85E-12;epsr=4;m=.25*9.1e-31;
mu=0;kT=.025;n0=m*kT*q/(2*pi*(hbar^2));

%inputs
a=3e-10;t0=(hbar^2)/(2*m*(a^2)*q);e0=q*a/eps0;
Nox=7;Nc=10;%use Nc=10,30 for 3,9nm channel respectively
Np=Nox+Nc+Nox;XX=a*1e9*[1:1:Np];
Ec=[3*ones(Nox,1);0*ones(Nc,1);3*ones(Nox,1)];

%Hamiltonian matrix
T=(2*t0*diag(ones(1,Np)))-(t0*diag(ones(1,Np-1),1))-(t0*diag(ones(1,Np-1),-1));

%dielectric constant matrix
D2=epsr*((2*diag(ones(1,Np)))-(diag(ones(1,Np-1),1))-(diag(ones(1,Np-1),-1)));
iD2=inv(D2);

Vg=linspace(-.25,.25,26);
for kg=1:26
Ubdy=-epsr*[Vg(kg);zeros(Np-2,1);Vg(kg)];kg;
%Ubdy=-epsr*[0;zeros(Np-2,1);Vg(kg)];;%for asymmetric bias
U0=iD2*Ubdy;

%self-consistent calculation
    U1=1e-6*ones(Np,1);UU=U1;change=1;
    while change>1e-3
        U1=U1+(0.1*(UU-U1));
        [P,D]=eig(T+diag(Ec)+diag(U1));D=diag(D);
        rho=log(1+exp((mu-D)./kT));rho=P*diag(rho)*P';
        n=2*n0*diag(rho);
            for kp=1:Np
                ncl(kp)=a*2*(n0^1.5)*Fhalf((mu-Ec(kp)-U1(kp))/kT);
            end
            %n=ncl';%use for semiclassical calculation
            UU=U0+(iD2*e0*n);
            change=max(max((abs(UU-U1))));
        U=Ec+U1;%self-consistent band profile
end
```

```
%electron density in channel per cm2
      ns(kg)=1e-4*sum(sum(n.*[zeros(Nox,1);ones(Nc,1);zeros(Nox,1)]));
            nn(:,kg)=1e-6*n./a;%electron density per cm3
            Fn(:,kg)=mu*ones(Nc+Nox+Nox,1);
end
C=q*(ns(26)-ns(25))/(Vg(26)-Vg(25));
d=1e-4*epsr*eps0*2/C;d,C
%ns=log10(ns)

hold on
h=plot(Vg,ns,'b');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
xlabel(' Vg (V) ---> ')
ylabel(' ns (/cm2) ---> ')
%axis([0 .3 0 3.5e12])
grid on
```

% Fig.7.3.2

```
clear all

E=linspace(-.5,1,1001);
D=sqrt(E);

hold on
h=plot(D,E,'b');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
xlabel(' D ( E ) (arb. units) ')
ylabel(' E ( eV ) ')
grid on
```

% Fig.7.3.4

```
clear all

E=linspace(-.25,.25,501);dE=E(2)-E(1);kT=0.025;Ef=0;
V=0;mu1=Ef+(V/2);mu2=Ef-(V/2);
f1=1./(1+exp((E-mu1)./kT));f2=1./(1+exp((E-mu2)./kT));
FT=[0 diff(f1)];FT=FT.*(-1/dE);
%dE*(sum(f1-f2))/V

hold on
h=plot(FT,E,'b');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
grid on
```

```
% Fig.7.4.1, Fig.7.4.2

clear all

z=zeros(5);Z=zeros(10);
%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;q=1.602e-19;a=2.45e-10*4/sqrt(3);m=9.110e-31;
d1=[1 1 1]/4;d2=[1 -1 -1]/4;d3=[-1 1 -1]/4;d4=[-1 -1 1]/4;

%sp3s* model parameters
soa=.3787/3;soc=.0129/3;
Esa=-8.3431;Epa=1.0414;Esc=-2.6569;Epc=3.6686;Esea=8.5914;Esec=6.7386;
Vss=-6.4513;Vpasc=-5.7839;Vpasec=-4.8077;
Vsapc=4.4800;Vseapc=4.8422;Vxx=1.9546;Vxy=5.0779;

%Valence band Luttinger-Kohn parameters
Ev=-.1;del=.3;g1=6.85;g2=2.1;g3=2.9;
t1=(hbar^2)*g1/(2*m*q*(a^2));
t2=(hbar^2)*g2/(2*m*q*(a^2));
t3=(hbar^2)*g3/(2*m*q*(a^2));

Nt=101;kk=1*linspace(0,1,Nt);
l=1;m=0;n=0;%X-direction
l=0.5;m=0.5;n=0.5;%L-direction

for Nk=1:Nt
k=2*pi*kk(Nk)*[l m n];

%sp3s* model
    p1=exp(i*sum(k.*d1));p2=exp(i*sum(k.*d2));
    p3=exp(i*sum(k.*d3));p4=exp(i*sum(k.*d4));
        g0=(p1+p2+p3+p4)/4;g1=(p1+p2-p3-p4)/4;
        g2=(p1-p2+p3-p4)/4;g3=(p1-p2-p3+p4)/4;

a1=diag([Esa Epa Epa Epa Esea]);A1=[a1 z;z a1];
a2=diag([Esc Epc Epc Epc Esec]);A2=[a2 z;z a2];
b=[Vss*g0 Vsapc*g1 Vsapc*g2 Vsapc*g3 0;
    Vpasc*g1   Vxx*g0 Vxy*g3 Vxy*g2 Vpasec*g1;
    Vpasc*g2 Vxy*g3 Vxx*g0 Vxy*g1 Vpasec*g2;
    Vpasc*g3 Vxy*g2 Vxy*g1 Vxx*g0 Vpasec*g3;
    0 Vseapc*conj(g1) Vseapc*conj(g2) Vseapc*conj(g3) 0];B=[b z;z b];
    h=[a1 b;b' a2];H=[A1 B;B' A2];

aso=soa*[0 0 0 0 0 0 0 0 0 0;
                0 0 -i 0 0 0 0 0 1 0;
                0 i 0 0 0 0 0 0 -i 0;
                0 0 0 0 0 0 -1 i 0 0;
                0 0 0 0 0 0 0 0 0 0;
                0 0 0 0 0 0 0 0 0 0;
                0 0 0 -1 0 0 0 i 0 0;
                0 0 0 -i 0 0 -i 0 0 0;
```

```
                0 1 i 0 0 0 0 0 0 0;
                0 0 0 0 0 0 0 0 0 0];
        cso=soc*[0 0 0 0 0 0 0 0 0 0;
                0 0 -i 0 0 0 0 0 1 0;
                0 i 0 0 0 0 0 0 -i 0;
                0 0 0 0 0 0 -1 i 0 0;
                0 0 0 0 0 0 0 0 0 0;
                0 0 0 0 0 0 0 0 0 0;
                0 0 0 -1 0 0 0 i 0 0;
                0 0 0 -i 0 0 -i 0 0 0;
                0 1 i 0 0 0 0 0 0 0;
                0 0 0 0 0 0 0 0 0 0];H=H+[aso Z;Z cso];

[V,D]=eig(H);
        eiglst = sum(D);
        E(Nk,:) = sort(real(eiglst));

%Valence band Luttinger-Kohn model
P=Ev+(t1*sum(k.*k));Q=t2*((k(1)^2)+(k(2)^2)-(2*(k(3)^2)));
R=-(sqrt(3)*t2*((k(1)^2)-(k(2)^2)))+(i*2*t3*sqrt(3)*k(1)*k(2));
S=2*t3*sqrt(3)*((k(1)-(i*k(2)))*k(3));

H4=-[P+Q -S R 0;
                -S' P-Q 0 R;
                R' 0 P-Q S;
                0 R' S' P+Q];[V,D]=eig(H4);
        eiglst = sum(D);
        ELK4(Nk,:) = sort(real(eiglst));

H6=-[P+Q -S R 0 -S/sqrt(2) sqrt(2)*R;
        -S' P-Q 0 R -sqrt(2)*Q sqrt(1.5)*S;
        R' 0 P-Q S sqrt(1.5)*S' sqrt(2)*Q;
        0 R' S' P+Q -sqrt(2)*R' -S'/sqrt(2);
        -S'/sqrt(2) -sqrt(2)*Q' sqrt(1.5)*S -sqrt(2)*R P+del 0;
        sqrt(2)*R' sqrt(1.5)*S' sqrt(2)*Q' -S/sqrt(2) 0 P+del];
                [V,D]=eig(H6);
        eiglst = sum(D);
        ELK6(Nk,:) = sort(real(eiglst));
end

kk=-kk;%L-direction

hold on
h1=plot(kk,E,'b');
%h2=plot(kk,ELK4,'b--');% Fig.6.4.1
h2=plot(kk,ELK6,'b--');% Fig.6.4.2
set(h1,'linewidth',[2.0])
set(h2,'linewidth',[3.0])
set(gca,'Fontsize',[24])
xlabel(' ka (fraction of maximum value) ---> ')
```

```
ylabel(' Energy ( eV ) ---> ')
axis([-1 1 -2 3])
grid on
```

% Fig.7.4.4

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;q=1.602e-19;a=3e-10;m=9.110e-31;

Eb=.15;
%Luttinger-Kohn parameters
g1=6.85;g2=2.1;g3=2.9;%GaAs
w1=(hbar^2)*g1/(2*m*q*(a^2));
w2=(hbar^2)*g2/(2*m*q*(a^2));
w3=(hbar^2)*g3/(2*m*q*(a^2));
    g1=3.45;g2=0.68;g3=1.29;%AlAs
    a1=(hbar^2)*g1/(2*m*q*(a^2));b1=(.7*w1)+(.3*a1);
    a2=(hbar^2)*g2/(2*m*q*(a^2));b2=(.7*w2)+(.3*a2);
    a3=(hbar^2)*g3/(2*m*q*(a^2));b3=(.7*w3)+(.3*a3);
Ev=0;Evb=(0.7*0)+(0.3*0.75);kx=0*pi;ky=0*pi;k2=(kx^2)+(ky^2);

for nk=1:20
Nw=nk+10;Nb=Nw;Np=Nb+Nw+Nb;W(nk)=(Nw-1)*a*1e9;Z=zeros(Np);nk
X(nk)=Nw-1;
t=[b1*ones(1,Nb) w1*ones(1,Nw-1) b1*ones(1,Nb)];tt=[0 t]+[t 0];
Ebk=Evb+(b1*k2);Ewk=(w1*k2);Ebwk=(Ebk+Ewk)/2;
U=Ev+[Ebk*ones(1,Nb) Ebwk Ewk*ones(1,Nw-2) Ebwk Ebk*ones(1,Nb)];
P=-diag(t,1)-diag(t,-1)+diag(tt)+diag(U);

t=-2*[b2*ones(1,Nb) w2*ones(1,Nw-1) b2*ones(1,Nb)];tt=[0 t]+[t 0];
Ebk=b2*k2;Ewk=w2*k2;Ebwk=(Ebk+Ewk)/2;
U=[Ebk*ones(1,Nb) Ebwk Ewk*ones(1,Nw-2) Ebwk Ebk*ones(1,Nb)];
Q=-diag(t,1)-diag(t,-1)+diag(tt)+diag(U);

Ebk=-(sqrt(3)*b2*((kx^2)-(ky^2)))+(i*2*b3*sqrt(3)*kx*ky);
Ewk=-(sqrt(3)*w2*((kx^2)-(ky^2)))+(i*2*w3*sqrt(3)*kx*ky);
Ebwk=(Ebk+Ewk)/2;
U=[Ebk*ones(1,Nb) Ebwk Ewk*ones(1,Nw-2) Ebwk Ebk*ones(1,Nb)];
R=diag(U);

t=2*i*sqrt(3)*(kx-(i*ky))*[b3*ones(1,Nb) w3*ones(1,Nw-1) b3*ones(1,Nb)];
S=diag(t,1)-diag(t,-1);

H=[P+Q Z;Z P+Q];HL=[P-Q Z;Z P-Q];
HC=[-S R;R' S'];
    H=-[H HC;HC' HL];

[V,D]=eig(H);D=diag(D);D=-(sort(real(-D)))';
E1(nk)=D(1);E2(nk)=D(2);E3(nk)=D(3);E4(nk)=D(4);
```

```
E5(nk)=D(5);E6(nk)=D(6);E7(nk)=D(7);E8(nk)=D(8);
end

%Analytical results for infinite well
Ean1=-(w1-(2*w2))*(pi^2)./(X.^2);
Ean2=-(w1+(2*w2))*(pi^2)./(X.^2);

hold on
%h=plot(W,Ean1,'b');
%h=plot(W,Ean2,'b');
h=plot(W,E1,'b');
%h=plot(W,E2,'bx');
h=plot(W,E3,'b');
%h=plot(W,E4,'b+');
h=plot(W,E5,'b');
%h=plot(W,E6,'bx');
h=plot(W,E7,'b');
%h=plot(W,E8,'b+');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
xlabel(' W ( nm ) ---> ')
ylabel(' Energy ( eV ) ---> ')
axis([3 9 -.25 0])
grid on
```

% Fig.7.4.5

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;q=1.602e-19;a=3e-10;m=9.110e-31;

%Luttinger-Kohn parameters
g1=6.85;g2=2.1;g3=2.9;%GaAs
w1=(hbar^2)*g1/(2*m*q*(a^2));
w2=(hbar^2)*g2/(2*m*q*(a^2));
w3=(hbar^2)*g3/(2*m*q*(a^2));
      g1=3.45;g2=0.68;g3=1.29;%AlAs
      a1=(hbar^2)*g1/(2*m*q*(a^2));b1=(.7*w1)+(.3*a1);
      a2=(hbar^2)*g2/(2*m*q*(a^2));b2=(.7*w2)+(.3*a2);
      a3=(hbar^2)*g3/(2*m*q*(a^2));b3=(.7*w3)+(.3*a3);
Ev=0;Evb=(0.7*0)+(0.3*0.75);

Nw=18;Nb=Nw;Np=Nb+Nw+Nb;W=(Nw-1)*a*1e9,Z=zeros(Np);

for nk=1:26
k(nk)=(nk-1)/500;% in A^-1
l=0;m=1;lm=sqrt((l^2)+(m^2));
kx=(l/lm)*k(nk)*a*1e10;ky=(m/lm)*k(nk)*a*1e10;
k2=(kx^2)+(ky^2);
```

```
t=[b1*ones(1,Nb) w1*ones(1,Nw-1) b1*ones(1,Nb)];tt=[0 t]+[t 0];
Ebk=Evb+(b1*k2);Ewk=(w1*k2);Ebwk=(Ebk+Ewk)/2;
U=Ev+[Ebk*ones(1,Nb) Ebwk Ewk*ones(1,Nw-2) Ebwk Ebk*ones(1,Nb)];
P=-diag(t,1)-diag(t,-1)+diag(tt)+diag(U);

t=-2*[b2*ones(1,Nb) w2*ones(1,Nw-1) b2*ones(1,Nb)];tt=[0 t]+[t 0];
Ebk=b2*k2;Ewk=w2*k2;Ebwk=(Ebk+Ewk)/2;
U=[Ebk*ones(1,Nb) Ebwk Ewk*ones(1,Nw-2) Ebwk Ebk*ones(1,Nb)];
Q=-diag(t,1)-diag(t,-1)+diag(tt)+diag(U);

Ebk=-(sqrt(3)*b2*((kx^2)-(ky^2)))+(i*2*b3*sqrt(3)*kx*ky);
Ewk=-(sqrt(3)*w2*((kx^2)-(ky^2)))+(i*2*w3*sqrt(3)*kx*ky);
Ebwk=(Ebk+Ewk)/2;
U=[Ebk*ones(1,Nb) Ebwk Ewk*ones(1,Nw-2) Ebwk Ebk*ones(1,Nb)];
R=diag(U);

t=-2*i*sqrt(3)*(kx-(i*ky))*[b3*ones(1,Nb) w3*ones(1,Nw-1) b3*ones(1,Nb)]/2;
S=diag(t,1)-diag(t,-1);

H=[P+Q Z;Z P+Q];HL=[P-Q Z;Z P-Q];
HC=[-S R;R' S'];
        H=-[H HC;HC' HL];
[nk sum(sum(abs(H-H')))]

[V,D]=eig(H);D=diag(D);D=-(sort(real(-D)))';
E1(nk)=D(1);E2(nk)=D(2);E3(nk)=D(3);E4(nk)=D(4);
end

k=k*10;%per Angstrom to per nm
hold on
%h=plot(W,Ean1,'b');
%h=plot(W,Ean2,'b');
h=plot(k,E1,'b');
%h=plot(k,E2,'bx');
h=plot(k,E3,'b');
%h=plot(k,E4,'b+');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
xlabel(' k ( /nm ) ---> ')
ylabel(' Energy ( eV ) ---> ')
axis([0 .5 -.1 0])
grid on
```

Chapter 8

% Fig.8.1

```
clear all

E=linspace(-.3,.3,50001);dE=E(2)-E(1);gam=0.05;
D=(gam/(2*pi))./(((E-.14).^2)+((gam/2)^2));
```

```
D=D+(gam/(2*pi))./(((E-.04).^2)+((gam/2)^2));%Use for Fig.P.5.2
D=D+((gam/(2*pi))./(((E+.06).^2)+((gam/2)^2)));%Use for Fig.P.5.2
D=D+(gam/(2*pi))./(((E+.15).^2)+((gam/2)^2));
dE*sum(D)

hold on
h=plot(D,E,'b');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
xlabel(' D(E) (per eV) --->')
ylabel(' E (eV) ---> ')
grid on
```

% Fig.8.2.5

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;m=0.25*9.1e-31;mu=0.25;kT=0.025;

%inputs
a=2e-10;t0=(hbar^2)/(2*m*(a^2)*q);Np=50;t0
X=a*linspace(0,Np-1,Np);U=linspace(-0.05,0.05,Np);
H=(2*t0*diag(ones(1,Np)))-(t0*diag(ones(1,Np-1),1))-(t0*diag(ones(1,Np-1),-1));
H=H+diag(U);HP=H;
HP(1,Np)=-t0;HP(Np,1)=-t0;

[V,D]=eig(HP);D=diag(D);
rho=1./(1+exp((D-mu)./kT));
rho=V*diag(rho)*V';rho=diag(rho)/a;

%Energy grid for Green's function method
Emin=-0.1;Emax=0.4;NE=250;E=linspace(Emin,Emax,NE);dE=E(2)-E(1);zplus=i*1e-12;
f=1./(1+exp((E-mu)./kT));

%Green's function method
sig1=zeros(Np,Np);sig2=zeros(Np,Np);n=zeros(Np,1);
    for k=1:NE
        ck=(1-((E(k)+zplus-U(1))/(2*t0)));ka=acos(ck);
            sigma=-t0*exp(i*ka);sig1(1,1)=sigma;
        ck=(1-((E(k)+zplus-U(Np))/(2*t0)));ka=acos(ck);
            sigma=-t0*exp(i*ka);sig2(Np,Np)=sigma;
            G=inv(((E(k)+zplus)*eye(Np))-H-sig1-sig2);
            n=n+(f(k)*(dE*diag(i*(G-G'))/(2*pi*a)));
    end

hold on
h=plot(X,rho,'b');
h=plot(X,n,'bx');
grid on
set(h,'linewidth',[2.0])
```

```
set(gca,'Fontsize',[24])
xlabel(' X ( m ) --> ')
ylabel(' n ( / m ) --> ')
```

% Fig.8.2.6

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;m=0.25*9.1e-31;mu=0.25;kT=0.025;

%inputs
a=2e-10;t0=(hbar^2)/(2*m*(a^2)*q);Np=50;t0
X=a*linspace(0,Np-1,Np);U=linspace(-0.05,0.05,Np);
H=(2*t0*diag(ones(1,Np)))-(t0*diag(ones(1,Np-1),1))-(t0*diag(ones(1,Np-1),-1));
H=H+diag(U);

%Energy grid for Green's function method
Emin=-0.1;Emax=0.4;NE=250;E=linspace(Emin,Emax,NE);dE=E(2)-E(1);zplus=i*1e-12;
f=1./(1+exp((E-mu)./kT));

%Green's function method
sig1=zeros(Np,Np);sig2=zeros(Np,Np);
    for k=1:NE
        ck=(1-((E(k)+zplus-U(1))/(2*t0)));ka=acos(ck);
            sigma=-t0*exp(i*ka);sig1(1,1)=sigma;
        ck=(1-((E(k)+zplus-U(Np))/(2*t0)));ka=acos(ck);
            sigma=-t0*exp(i*ka);sig2(Np,Np)=sigma;
            G=inv(((E(k)+zplus)*eye(Np))-H-sig1-sig2);
            D0=diag(i*(G-G'))/(2*pi);D1(k)=D0(1);D2(k)=D0(Np);
    end

hold on
%h=plot(X,U,'b');
h=plot(D1,E,'b');
%h=plot(D2,E,'b');
grid on
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
xlabel(' X ( m ) --> ')
ylabel(' U ( eV ) --> ')
%axis([0 1e-8 -.1 .4])
axis([0 1.2 -.1 .4])
```

%Fig.8.4.1

```
ep=-0.25;ep1=0.25;t=0.5;eta=0.025;
H=[ep t;t ep1];

E=linspace(-1,1,201);
for kE=1:201
```

```
G=inv(((E(kE)+(i*eta))*eye(2,2))-H);
A=diag(i*(G-G'));D(kE)=A(1);
end

hold on
h=plot(D,E,'gx');
set(h,'linewidth',[3.0])
set(gca,'Fontsize',[24])
grid on
xlabel(' LDOS (/ eV) –> ')
ylabel(' Energy (eV) –> ')
```

%Fig.E.8.2

```
clear all
t0=1;zplus=1e-10;

NE=81;X=linspace(-1,3,NE);
for kE=1:NE
    E=2*X(kE);
    ck=1-((E+zplus)/(2*t0));ka=acos(ck);
    if imag(ka) < 0
        ka=ka';end
    sig(kE)=-t0*exp(i*ka);
end

hold on
h1=plot(real(sig),X,'g');
h2=plot(imag(sig),X,'g');
h1=plot(real(sig),X,'go');
set(h1,'linewidth',[2.0])
set(h2,'linewidth',[4.0])
set(gca,'Fontsize',[24])
grid on
xlabel(' --> ')
ylabel(' --> ')
```

%Fig. E.8.5

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;m=0.25*9.1e-31;zplus=i*5e-3;

%inputs
a=2.5e-10;t0=(hbar^2)/(2*m*(a^2)*q);Np=100;t0
X=a*linspace(0,Np-1,Np);U=zeros(1,Np);U(Np/2)=5/(a*1e10);
H=(2*t0*diag(ones(1,Np)))-(t0*diag(ones(1,Np-1),1))-(t0*diag(ones(1,Np-1),-1));
H=H+diag(U);
E=0.1;
```

```
%Green's function method
sig1=zeros(Np,Np);sig2=zeros(Np,Np);
      ck=(1-((E+zplus-U(1))/(2*t0)));ka=acos(ck);
            sigma=-t0*exp(i*ka);sig1(1,1)=sigma;
      ck=(1-((E+zplus-U(Np))/(2*t0)));ka=acos(ck);
            sigma=-t0*exp(i*ka);sig2(Np,Np)=sigma;
                  G=inv(((E+zplus)*eye(Np))-H-sig1-sig2);
                  D0=diag(i*(G-G'))/(2*pi);

hold on
h=plot(X,D0,'b');
grid on
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
xlabel(' X (m) --> ')
ylabel(' DOS ( / eV ) --> ')
```

Chapter 9

% Fig.9.4.2

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.055e-34;m=9.110e-31;q=1.602e-19;a=5e-10;L=10e-9;

k=0.5*linspace(-1,1,201)/a;
Ek=(hbar^2)*(k.^2)/(2*0.25*m*q);
EE=linspace(0,0.2,201);

%Subband (1,1)
E1=2*(hbar^2)*(pi^2)/(2*0.25*m*q*L^2);
M=((EE-E1)+abs(EE-E1))./(2*abs(EE-E1));

%Subbands (1,2) and (2,1)
E2=5*(hbar^2)*(pi^2)/(2*0.25*m*q*L^2);
M=M+(((EE-E2)+abs(EE-E2))./(abs(EE-E2)));

%Subband (2,2)
E3=8*(hbar^2)*(pi^2)/(2*0.25*m*q*L^2);
M=M+(((EE-E3)+abs(EE-E3))./(2*abs(EE-E3)));
k=k*1e-9;
hold on
h=plot(k,E1+Ek,'b');
h=plot(k,E2+Ek,'b');
h=plot(k,E3+Ek,'b');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
xlabel('k ( / nm )');
ylabel('E - Ec ( eV ) -->');
axis([-1 1 0 0.3]);
grid on
```

% Fig.9.5.5

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;m=.25*9.1e-31;IE=(q*q)/(2*pi*hbar);
Ef=0.1;kT=.025;

%inputs
a=3e-10;t0=(hbar^2)/(2*m*(a^2)*q);
NS=15;NC=30;ND=15;Np=NS+NC+ND;

%Hamiltonian matrix
%NS=15;NC=20;ND=15;Np=NS+NC+ND;UB=0*ones(Np,1);%no barrier
%NS=23;NC=4;ND=23;Np=NS+NC+ND;
    %UB=[zeros(NS,1);0.4*ones(NC,1);zeros(ND,1);];%tunneling barrier
NS=15;NC=16;ND=15;Np=NS+NC+ND;
    UB=[zeros(NS,1);.4*ones(4,1);zeros(NC-8,1);.4*ones(4,1);zeros(ND,1)];%RT barrier
T=(2*t0*diag(ones(1,Np)))-(t0*diag(ones(1,Np-1),1))-(t0*diag(ones(1,Np-1),-1));
T=T+diag(UB);

%Bias
V=0;mu1=Ef+(V/2);mu2=Ef-(V/2);
U1=V*[.5*ones(1,NS) linspace(0.5,-0.5,NC) -.5*ones(1,ND)];
U1=U1';%Applied potential profile

%Energy grid for Green's function method
NE=501;E=linspace(-.2,.8,NE);zplus=i*1e-12;dE=E(2)-E(1);
    f1=1./(1+exp((E-mu1)./kT));
        f2=1./(1+exp((E-mu2)./kT));

%Transmission
I=0;%Current
for k=1:NE
    sig1=zeros(Np);sig2=zeros(Np);sig3=zeros(Np);
    ck=1-((E(k)+zplus-U1(1)-UB(1))/(2*t0));ka=acos(ck);
    sig1(1,1)=-t0*exp(i*ka);gam1=i*(sig1-sig1');
        ck=1-((E(k)+zplus-U1(Np)-UB(Np))/(2*t0));ka=acos(ck);
        sig2(Np,Np)=-t0*exp(i*ka);gam2=i*(sig2-sig2');
            G=inv(((E(k)+zplus)*eye(Np))-T-diag(U1)-sig1-sig2-sig3);
                TM(k)=real(trace(gam1*G*gam2*G'));
                    I=I+(dE*IE*TM(k)*(f1(k)-f2(k)));
end
V,I

XX=a*1e9*[1:1:Np];
XS=XX([1:NS-4]);XD=XX([NS+NC+5:Np]);

hold on
%h=plot(TM,E,'b');
h=plot(XX,U1+UB,'b');
h=plot(XS,mu1*ones(1,NS-4),'b--');
```

```
h=plot(XD,mu2*ones(1,ND-4),'b--');
%axis([0 1.1 -.2 .8])
axis([0 15 -.2 .8])
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
%xlabel(' Transmission ---> ')
xlabel(' z ( nm ) --->')
ylabel(' Energy ( eV ) ---> ')
grid on
```

% Fig.9.5.8

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;m=.25*9.1e-31;IE=(q*q)/(2*pi*hbar);
Ef=0.1;kT=.025;

%inputs
a=3e-10;t0=(hbar^2)/(2*m*(a^2)*q);
NS=15;NC=30;ND=15;Np=NS+NC+ND;

%Hamiltonian matrix
NS=15;NC=16;ND=15;Np=NS+NC+ND;
    UB=[zeros(NS,1);.4*ones(4,1);zeros(NC-8,1);.4*ones(4,1);zeros(ND,1)];%RT barrier
T=(2*t0*diag(ones(1,Np)))-(t0*diag(ones(1,Np-1),1))-(t0*diag(ones(1,Np-1),-1));
T=T+diag(UB);

%Bias
V=0;mu1=Ef+(V/2);mu2=Ef-(V/2);
U1=V*[.5*ones(1,NS) linspace(0.5,-0.5,NC) -.5*ones(1,ND)];
U1=U1';%Applied potential profile

%Energy grid for Green's function method
NE=501;E=linspace(-.2,.8,NE);zplus=i*1e-12;dE=E(2)-E(1);
    f1=1./(1+exp((E-mu1)./kT));
        f2=1./(1+exp((E-mu2)./kT));

%Transmission
I=0;%Current
for k=1:NE
    sig1=zeros(Np);sig2=zeros(Np);sig3=zeros(Np);
    ck=1-((E(k)+zplus-U1(1)-UB(1))/(2*t0));ka=acos(ck);
    sig1(1,1)=-t0*exp(i*ka);gam1=i*(sig1-sig1');
        ck=1-((E(k)+zplus-U1(Np)-UB(Np))/(2*t0));ka=acos(ck);
        sig2(Np,Np)=-t0*exp(i*ka);gam2=i*(sig2-sig2');
            sig3(Np/2,Np/2)=-i*0.25;gam3=i*(sig3-sig3');%Büttiker probe
            G=inv(((E(k)+zplus)*eye(Np))-T-diag(U1)-sig1-sig2-sig3);
                T12=real(trace(gam1*G*gam2*G'));
                T13=real(trace(gam1*G*gam3*G'));
```

```
                T23=real(trace(gam2*G*gam3*G'));
                    TM(k)=T12+(T13*T23/(T12+T23));
                        I=I+(dE*IE*TM(k)*(f1(k)-f2(k)));
end
V,I

XX=a*1e9*[1:1:Np];
XS=XX([1:NS-4]);XD=XX([NS+NC+5:Np]);

hold on
h=plot(TM,E,'b');
axis([0 1.1 -.2 .8])
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
xlabel(' Transmission ---> ')
ylabel(' Energy ( eV ) ---> ')
grid on
```

% Fig.9.5.10

```
clear all

%Constants (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;m=.25*9.1e-31;IE=(q*q)/(2*pi*hbar);
Ef=0.1;kT=.025;

%inputs
a=3e-10;t0=(hbar^2)/(2*m*(a^2)*q);
NS=15;NC=30;ND=15;Np=NS+NC+ND;
%Hamiltonian matrix
%NS=15;NC=20;ND=15;Np=NS+NC+ND;UB=0*ones(Np,1);%no barrier
%NS=23;NC=4;ND=23;Np=NS+NC+ND;
    %UB=[zeros(NS,1);0.4*ones(NC,1);zeros(ND,1);];%tunneling barrier
NS=15;NC=16;ND=15;Np=NS+NC+ND;
    UB=[zeros(NS,1);0.4*ones(4,1);zeros(NC-8,1);0.4*ones(4,1);zeros(ND,1)];%RT barrier
T=(2*t0*diag(ones(1,Np)))-(t0*diag(ones(1,Np-1),1))-(t0*diag(ones(1,Np-1),-1));
T=T+diag(UB);

%Bias
NV=26;VV=linspace(0,.5,NV);
for iV=1:NV
V=VV(iV);mu1=Ef+(V/2);mu2=Ef-(V/2);
U1=V*[.5*ones(1,NS) linspace(0.5,-0.5,NC) -.5*ones(1,ND)];
U1=U1';%Applied potential profile

%Energy grid for Green's function method
NE=101;E=linspace(-.2,.8,NE);zplus=i*1e-12;dE=E(2)-E(1);
    f1=1./(1+exp((E-mu1)./kT));
    f2=1./(1+exp((E-mu2)./kT));
        %For infinite 2-D cross-section
```

```
                %f1=(2*m*kT*q/(2*pi*hbar^2)).*log(1+exp((mu1-E)./kT));
                %f2=(2*m*kT*q/(2*pi*hbar^2)).*log(1+exp((mu2-E)./kT));

%Transmission
I=0;%Current
for k=1:NE
    sig1=zeros(Np);sig2=zeros(Np);sig3=zeros(Np);
    ck=1-((E(k)+zplus-U1(1)-UB(1))/(2*t0));ka=acos(ck);
    sig1(1,1)=-t0*exp(i*ka);gam1=i*(sig1-sig1');
        ck=1-((E(k)+zplus-U1(Np)-UB(Np))/(2*t0));ka=acos(ck);
        sig2(Np,Np)=-t0*exp(i*ka);gam2=i*(sig2-sig2');
            sig3(Np/2,Np/2)=-i*0.00025;gam3=i*(sig3-sig3');%Büttiker probe
            G=inv(((E(k)+zplus)*eye(Np))-T-diag(U1)-sig1-sig2-sig3);
                T12=real(trace(gam1*G*gam2*G'));
                T13=real(trace(gam1*G*gam3*G'));
                T23=real(trace(gam2*G*gam3*G'));
                    TM(k)=T12+(T13*T23/(T12+T23));
                        I=I+(dE*IE*TM(k)*(f1(k)-f2(k)));
end
II(iV)=I;V,I
end

XX=a*1e9*[1:1:Np];
XS=XX([1:NS-4]);XD=XX([NS+NC+5:Np]);

hold on
h=plot(VV,II,'b');
%h=plot(XX,U1+UB,'b');
%h=plot(XS,mu1*ones(1,NS-4),'b--');
%h=plot(XD,mu2*ones(1,ND-4),'b--');
axis([0 .5 0 3.5e-7])
%axis([0 15 -.3 .7])
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
xlabel(' Voltage ( V ) ---> ')
%xlabel(' z ( nm ) --->')
%ylabel(' Energy ( eV ) ---> ')
ylabel(' Current ( A ) ---> ')
grid on
```

Chapter 10

% Fig.10.4.4

```
clear all

beta=pi*linspace(-1,1,201);w0=1;
y=sqrt(2*w0*(1-cos(beta)));

hold on
h=plot(beta,y,'b');
```

```
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
grid on
```

% Fig.10.4.5

```
clear all

beta=pi*linspace(-1,1,201);w1=1;w2=2;
for n=1:201
    A=[w1+w2 w1+(w2*exp(-i*beta(n)));w1+(w2*exp(i*beta(n))) w1+w2];
    [V,D]=eig(A);D=sort(real(diag(D)));
    D1(n)=real(sqrt(D(1)));D2(n)=real(sqrt(D(2)));
end

hold on
h=plot(beta,D1,'b');
h=plot(beta,D2,'b');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
grid on
```

Chapter 11

% Fig.11.2.2, 11.2.7

```
clear all

%1-D with elastic phase-breaking and/or coherent, T vs. E, fixed length

%Constants (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;m=1*9.1e-31;IE=(q*q)/(2*pi*hbar);kT=.025;

%inputs
a=3e-10;t0=(hbar^2)/(2*m*(a^2)*q);D=0.01*0;

%Energy grid
NE=401;E=linspace(.1,.3,NE);zplus=i*1e-12;dE=E(2)-E(1);

%Bias
V=0.01;f1=1/(1+exp((-V/2)/kT));
        f2=1/(1+exp((V/2)/kT));

%Hamiltonian
    Np=40;UB=zeros(Np,1);UB(5)=0.5*1;UB(36)=0.5*1;
    U1=V*linspace(0.5,-0.5,Np)';XX=a*linspace(0,Np-1,Np);
    T=(2*t0*diag(ones(1,Np)))-(t0*diag(ones(1,Np-1),1))-(t0*diag(ones(1,Np-1),-1));

%Iterative solution
for k=1:NE
    sig1=zeros(Np);sig2=zeros(Np);
    ck=1-((E(k)+zplus-U1(1)-UB(1))/(2*t0));ka=acos(ck);
```

```
    sig1(1,1)=-t0*exp(i*ka);gam1=i*(sig1-sig1');
        ck=1-((E(k)+zplus-U1(Np)-UB(Np))/(2*t0));ka=acos(ck);
        sig2(Np,Np)=-t0*exp(i*ka);gam2=i*(sig2-sig2');

    %calculating the Green function, G self-consistently
    G=inv(((E(k)+zplus)*eye(Np))-T-diag(U1+UB)-sig1-sig2);change=1;
        while(change>1e-4)
            sigp=diag(D*diag(G));
    S=inv(((E(k)+zplus)*eye(Np))-T-diag(U1+UB)-sig1-sig2-sigp);
    change=sum(sum(abs(G-S)))/(sum(sum(abs(G)+abs(S))));
        G=(0.5*G)+(0.5*S);
        end
        G=S;A=i*(G-G');
        M=D*(G.*conj(G));

    %calculating the electron density,n(r;E)
    gamp=i*(sigp-sigp');gamma=gam1+gam2+gamp;
        sigin1=f1*gam1;sigin2=f2*gam2;
        n=(inv(eye(Np)-M))*diag(G*(sigin1+sigin2)*G');
        siginp=D*diag(n);

    %calculating the correlation function Gn
        Gn=G*(sigin1+sigin2+siginp)*G';
    %calculating the effective transmission
        I1(k)=(1/(f2-f1))*real(trace(gam1*Gn)-trace(sigin1*A));
        I2(k)=(1/(f1-f2))*real(trace(gam2*Gn)-trace(sigin2*A));
end

hold on
h=plot(I1,E,'b');
%h=plot(I2,E,'bx');
%h=plot(1e9*XX,U1+UB,'b');
%h=plot(1e9*XX,U1+UB,'bo');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
%xlabel(' x ( nm ) ---> ')
%ylabel(' Potential ( eV ) ---> ')
xlabel(' Transmission ---> ')
ylabel(' Energy ( eV ) ---> ')
grid on
axis([0 1.1 .1 .3])
```

% Fig.11.2.4, 11.2.6

```
clear all

%multi-moded coherent transport,T vs. E

%Constants (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;m=9.1e-31;IE=(q*q)/(2*pi*hbar);kT=.025;
```

```
%inputs
a=5e-10;t0=(hbarˆ2)/(2*m*(aˆ2)*q);
%Energy grid
NE=11;% 11 for one scatterer, 101 for two
E=linspace(0.1,0.3,NE);zplus=i*1e-12;dE=E(2)-E(1);

%Bias
V=0.01;f1=1/(1+exp((-V/2)/kT));
        f2=1/(1+exp((V/2)/kT));

%Transverse modes
NW=15;NT=7;
alpha=(4*t0*diag(ones(1,NW)))-(t0*diag(ones(1,NW-1),1))-(t0*diag(ones(1,NW-1),-1));
[VT,D]=eig(alpha);[D ind]=sort(diag(D));
in=[];for k=1:NT
   in=[in ind(k)];end
VT=VT(:,in);D=diag(VT'*alpha*VT);

%Hamiltonian
   Np=40;UB=zeros(Np,1);UB(5)=0.25*1;UB(36)=0.25*0;
   impshape=[linspace(0,1,7) linspace(1,0,NW-7)];
   U1=V*linspace(0.5,-0.5,Np)';
   al=alpha+(U1(1)*eye(NW,NW));
   H=VT'*al*VT;H1=H;
   Z=zeros(NT,NT);bet=-t0*eye(NT,NT);
   for N=2:Np
      al=alpha+(U1(N)*eye(NW,NW));al1=al;
      al=al+(diag(UB(N)*impshape));
      al=VT'*al*VT;H=[H bet;bet' al];
      al1=VT'*al1*VT;H1=[H1 bet;bet' al1];%Use for one scatterer
      bet=[Z;bet];
   end

%calculating the transmission
for k=1:NE
   ck=(D-E(k)-zplus+U1(1))./(2*t0);ka=acos(ck);
   s1=-t0*exp(i.*ka);sig1=[diag(s1) zeros(NT,NT*(Np-1));zeros(NT*(Np-1),NT*Np)];
      ck=(D-E(k)-zplus+U1(Np))./(2*t0);ka=acos(ck);
      s2=-t0*exp(i.*ka);sig2=[zeros(NT*(Np-1),NT*Np);zeros(NT,NT*(Np-1)) diag(s2);];
      gam1=i*(sig1-sig1');gam2=i*(sig2-sig2');

   G=inv(((E(k)+zplus)*eye(NT*Np))-H-sig1-sig2);
      T(k)=real(trace(gam1*G*gam2*G'));
   G1=inv(((E(k)+zplus)*eye(NT*Np))-H1-sig1-sig2);%Use for one scatterer
      M(k)=real(trace(gam1*G1*gam2*G1'));[k T(k) M(k)],%use for one scatterer
end

Tsc=T./(2-(T./M));%semiclassical addition, use for one scatterer

%save condfluct2
XX=a*linspace(0,Np-1,Np);
```

```
hold on
%h=plot(T,E,'b');
h=plot(Tsc,E,'b--');
%h=plot(M,E,'b');
set(h,'linewidth',[2.0]);
set(gca,'Fontsize',[24]);
xlabel(' Transmission ---> ')
ylabel(' Energy ( eV ) ---> ')
axis([0 5 .1 .3])
grid on
```

% Fig.11.2.8

```
clear all

%1-D elastic coherent and/or phase-breaking, R vs. L, fixed E

%Constants (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;m=.25*9.1e-31;IE=(q*q)/(2*pi*hbar);kT=.025;

%inputs
a=3e-10;t0=(hbar^2)/(2*m*(a^2)*q);D=0.05;V=0.01;

%Bias

%Energy grid
E=0.1;zplus=i*1e-12;
    f1=1/(1+exp((-V/2)/kT));
        f2=1/(1+exp((V/2)/kT));

%Current
for k=2:21
    Np=k;UB=zeros(Np,1);U1=V*linspace(0.5,-0.5,Np)';k
    T=(2*t0*diag(ones(1,Np)))-(t0*diag(ones(1,Np-1),1))-(t0*diag(ones(1,Np-1),-1));

    sig1=zeros(Np);sig2=zeros(Np);sig3=zeros(Np);
    ck=1-((E+zplus-U1(1)-UB(1))/(2*t0));ka=acos(ck);
    sig1(1,1)=-t0*exp(i*ka);gam1=i*(sig1-sig1');
        ck=1-((E+zplus-U1(Np)-UB(Np))/(2*t0));ka=acos(ck);
        sig2(Np,Np)=-t0*exp(i*ka);gam2=i*(sig2-sig2');

    %calculating the Green function, G self-consistently
    G=inv(((E+zplus)*eye(Np))-T-diag(U1+UB)-sig1-sig2);change=1;
        while(change>1e-4)
            sigp=diag(D*diag(G));
    S=inv(((E+zplus)*eye(Np))-T-diag(U1+UB)-sig1-sig2-sigp);
    change=sum(sum(abs(G-S)))/(sum(sum(abs(G)+abs(S))));
        G=(0.5*G)+(0.5*S);
        end
        G=S;A=i*(G-G');
        M=D*(G.*conj(G));
```

```
    %calculating the inscattering functions from the contacts F1,F2
    gam1=i*(sig1-sig1');gam2=i*(sig2-sig2');
    gamp=i*(sigp-sigp');gamma=gam1+gam2+gamp;
        sigin1=f1*gam1;sigin2=f2*gam2;
        n=(inv(eye(Np)-M))*diag(G*(sigin1+sigin2)*G');
        siginp=D*diag(n);

    %calculating the correlation function Gn
        Gn=G*(sigin1+sigin2+siginp)*G';

    %calculating the current
        I1(k-1)=(1/(f1-f2))*real(trace(gam1*Gn)-trace(sigin1*A));
        I2(k-1)=(1/(f1-f2))*real(trace(gam2*Gn)-trace(sigin2*A));
        L(k-1)=k*a*1e10;
end

L=L./10;% Angstrom to nm
hold on
h=plot(L,1./I2,'b');
%h=plot(I1+I2,'g--');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
xlabel(' Length ( nm ) ---> ')
ylabel(' Normalized resistance ---> ')
axis([0 6 0 3])
grid on
```

% Fig.11.3.1, 11.3.2, 11.3.3

```
clear all

%1-D with inelastic scattering

%Constants (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;m=.25*9.1e-31;Ef=0.15;kT=0.025;

%inputs
a=3e-10;t0=(hbar^2)/(2*m*(a^2)*q);

%Hamiltonian matrix
    Np=40;UB=0*[zeros(10,1);0.25*ones(Np-10,1)];
    T=(2*t0*diag(ones(1,Np)))-(t0*diag(ones(1,Np-1),1))-(t0*diag(ones(1,Np-1),-1));

%Bias
V=0.1;mu1=Ef+(V/2);mu2=Ef-(V/2);
U1=V*[.5*ones(1,1) linspace(0.5,-0.5,Np-2) -.5*ones(1,1)]';%Applied potential profile
    D=1e-1;%Scattering strength

%Energy grid
NE=101;E=linspace(-.05,.35,NE);zplus=i*1e-12;dE=E(2)-E(1);
    f1=1./(1+exp((E-mu1)./kT));
        f2=1./(1+exp((E-mu2)./kT));
```

```
%Initial guess
sigin=0*ones(Np,NE);sigout=0*ones(Np,NE);

%Iterative solution of transport equation
change=1;it=1;n=zeros(Np,NE);p=zeros(Np,NE);
while change>1e-3
for k=1:NE
    sig1=zeros(Np);sig2=zeros(Np);
        ck=1-((E(k)+zplus-U1(1)-UB(1))/(2*t0));ka=acos(ck);
        sig1(1,1)=-t0*exp(i*ka);gam1=i*(sig1-sig1');
            ck=1-((E(k)+zplus-U1(Np)-UB(Np))/(2*t0));ka=acos(ck);
            sig2(Np,Np)=-t0*exp(i*ka);gam2=i*(sig2-sig2');
        sigin1(:,k)=f1(k)*diag(gam1);sigin2(:,k)=f2(k)*diag(gam2);
        sigout1(:,k)=(1-f1(k))*diag(gam1);sigout2(:,k)=(1-f2(k))*diag(gam2);
        gamp=sigin(:,k)+sigout(:,k);

    G=inv(((E(k)+zplus)*eye(Np))-T-diag(U1+UB)-sig1-sig2+(i*0.5*diag(gamp)));
        A=diag(i*(G-G'));
        n(:,k)=real(diag(G*((f1(k)*gam1)+(f2(k)*gam2)+diag(sigin(:,k)))*G'));
        p(:,k)=A-n(:,k);
end

off=0;%less than NE-1, equal to 0 for elastic
C=exp(-dE*off/kT);
ne=n(:,[off+1:NE]);ne=[ne zeros(Np,off)];
na=n(:,[1:NE-off]);na=[zeros(Np,off) na];
pa=p(:,[off+1:NE]);pa=[pa zeros(Np,off)];
pe=p(:,[1:NE-off]);pe=[zeros(Np,off) pe];

siginnew=(D*ne)+(C*D*na);
sigoutnew=(D*pe)+(C*D*pa);
change=sum(sum(abs(siginnew-sigin)));
change=change+sum(sum(abs(sigoutnew-sigout)))
sigin=((1-it)*sigin)+(it*siginnew);
sigout=((1-it)*sigout)+(it*sigoutnew);
end

    I1=real((sigout1.*n)-(sigin1.*p));I1=sum(I1);
    I2=real((sigout2.*n)-(sigin2.*p));I2=sum(I2);
    I3=real((sigout.*n)-(sigin.*p));I3=sum(I3);

I123=(dE/V)*[sum(I1) sum(I2) sum(I3)],%Normalized Conductance
IE=(dE/(V*V))*[sum(E.*I1) sum(E.*I2) sum(E.*I3)],%Normalized Power
kirchoff=[sum(I123) sum(IE)],%checking for conservation of current and energy current

save inel0
hold on
h=plot(I1,E,'b');
h=plot(I2,E,'b--');
%h=plot(I3,E,'c');
set(h,'linewidth',[2.0])
```

```
set(gca,'Fontsize',[24])
xlabel(' Normalized current / energy ---> ')
ylabel(' Energy ( eV ) ---> ')
axis([-.2 .2 -.05 .35])
```

% Fig.11.4.4

```
clear all

%Ballistic self-consistent solution

%Constants (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;m=.25*9.1e-31;
kT=0.0259;zplus=i*1e-12;eps0=8.854e-12;

%inputs
a=3e-10;t0=(hbar^2)/(2*m*(a^2)*q);N=40;
Ef=0.1;Ec=-0.5;Vg=0;
r=5e-9;tox=5e-9;K=2;%Use large value of permittivity K for Laplace limit
U0=q/2/pi/a/K/eps0.*log((r+tox)/r)

%Hamiltonian matrix
    Np=40;
    H0=(2*t0*diag(ones(1,Np)))-(t0*diag(ones(1,Np-1),1))-(t0*diag(ones(1,Np-1),-1));

%Energy grid
    NE=401;E=linspace(-0.5,0.3,NE);dE=E(2)-E(1);I0=(q^2)/hbar/2/pi

%Bias
iV=41;V=linspace(0,0.4,iV);n0=0;UL=-Vg*ones(Np,1);U=UL;
for kk=1:iV
    Vd=V(kk);mu1=Ef;mu2=Ef-Vd;
    sig1=zeros(Np);sig2=zeros(Np);
    epsilon=1;
    while (epsilon>0.001)
        rho=0;
        for k=1:NE
            f1=1/(1+exp((E(k)-mu1)/kT));f2=1/(1+exp((E(k)-mu2)/kT));

            cka1=1-(E(k)+zplus-Ec)/2/t0; ka1=acos(cka1);
            sig1(1,1)=-t0*exp(i*ka1);gam1=i*(sig1-sig1');
                cka2=1-(E(k)+zplus-Ec+Vd)/2/t0; ka2=acos(cka2);
        sig2(N,N)=-t0*exp(i*ka2);gam2=i*(sig2-sig2');
                G=inv((E(k)+zplus)*eye(N)-H0-diag(U)-sig1-sig2);A=i*(G-G');
                    sigin1=f1*gam1;sigin2=f2*gam2;
                        Gn=G*(sigin1+sigin2)*G';rho=rho+dE/2/pi*Gn;
                T(k)=trace(gam1*G*gam2*G');
        I1(k)=real(trace(sigin1*A)-trace(gam1*Gn));
        I2(k)=-real(trace(sigin2*A)-trace(gam2*Gn));
            end
        n=real(diag(rho));Unew=UL+(U0*(n-n0));
```

```
    dU=Unew-U;epsilon=max(abs(dU))
    U=U+0.25*dU;
        if Vd==0
        n0=n;epsilon=0;end
    end
    ID1=2*I0*dE*sum(I1);ID2=2*I0*dE*sum(I2);%2 for spin
    I(kk)=ID1;
end

save IV2
IonL=I0*Ef
hold on
h=plot(V,I,'b');
h=plot(V,IonL*ones(iV,1),'bx');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
grid on
xlabel(' Voltage ( V ) --> ')
ylabel(' Current ( A ) --> ')
```

% Fig.E.11.5

```
clear all

%1-D tunneling and/or elastic phase-breaking, R vs. L, fixed E

%Constants (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;m=.25*9.1e-31;IE=(q*q)/(2*pi*hbar);kT=.025;
zplus=i*1e-51;

%inputs
a=3e-10;t0=(hbarˆ2)/(2*m*(aˆ2)*q);
D=3e-1;% Scattering Strength: 2e-1 (x's) and 3e-1 (o's) eVˆ2
V=0.001;% Applied voltage
mu=0.1;% Fermi energy
    f1=1/(1+exp((-V/2)/kT));%Fermi function in contact 1 at E=mu
        f2=1/(1+exp((V/2)/kT));%Fermi function in contact 2 at E-mu

% Actual calculation
E=mu;
for k=5:26
    Np=k;%Length of barrier = (Np-2)*a
    UB=[0;0.5*ones(Np-2,1);0];% Barrier height
    U1=V*linspace(0.5,-0.5,Np)';% Applied potential profile
    T=(2*t0*diag(ones(1,Np)))-(t0*diag(ones(1,Np-1),1))-...
        (t0*diag(ones(1,Np-1),-1));%Tight-binding Hamiltonian

    sig1=zeros(Np);sig2=zeros(Np);sig3=zeros(Np);
    ck=1-((E+zplus-U1(1)-UB(1))/(2*t0));ka=acos(ck);
    sig1(1,1)=-t0*exp(i*ka);gam1=i*(sig1-sig1');%Self-energy for contact 1
```

```
        ck=1-((E+zplus-U1(Np)-UB(Np))/(2*t0));ka=acos(ck);
        sig2(Np,Np)=-t0*exp(i*ka);gam2=i*(sig2-sig2');%Self-energy for contact 2

    %calculating the Green function, G self-consistently
    G=inv(((E+zplus)*eye(Np))-T-diag(U1+UB)-sig1-sig2);change=1;
        while(change>1e-15)
        sigp=diag(D*diag(G));%Self-energy due to scattering
    S=inv(((E+zplus)*eye(Np))-T-diag(U1+UB)-sig1-sig2-sigp);
    change=sum(sum(abs(G-S)))/(sum(sum(abs(G)+abs(S))));
        G=(0.5*G)+(0.5*S);
        end
        G=S;A=i*(G-G');M=D*(G.*conj(G));

    %calculating the inscattering functions from the contacts F1,F2
    gam1=i*(sig1-sig1');gam2=i*(sig2-sig2');
    gamp=i*(sigp-sigp');gamma=gam1+gam2+gamp;
        sigin1=f1*gam1;sigin2=f2*gam2;
        n=(inv(eye(Np)-M))*diag(G*(sigin1+sigin2)*G');
        siginp=D*diag(n);%Inflow due to scattering


    %calculating the correlation function Gn
        Gn=G*(sigin1+sigin2+siginp)*G';

    %calculating the current
        I1(k-4)=(1/(f1-f2))*real(trace(gam1*Gn)-trace(sigin1*A));
        I2(k-4)=(1/(f1-f2))*real(trace(gam2*Gn)-trace(sigin2*A));
        L(k-4)=(k-2)*a*1e9;%in nanometers
end

hold on
h=plot(L,log10(-1./I1),'g');% Current at left end
h=plot(L,log10(1./I2),'go');% Current at right end
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
xlabel(' Length ( nm ) ---> ')
ylabel(' log10 ( resistance ) ---> ')
grid on
```

%Fig.E.11.6

```
clear all
%0-D with inelastic scattering

%Constants (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;I0=q*q/(2*pi*hbar);

%Parameters
    H0=5;Ef=0;kT=0.0025;dE=0.0005;zplus=i*1e-12;gamma=0.1;
        D0=0;Dnu=0*[0.5 0.7];Nph=size(Dnu,2);
            hnu=[100 550];%Multiply by dE for actual hnu
                Nhnu=1./((exp(dE*hnu./kT))-1);
```

```
%Bias
NV=203;VV=linspace(-0.51,0.5,NV);dV=VV(2)-VV(1);
for iV=1:NV
V=VV(iV);mu1=Ef;mu2=Ef-V;U1=(-0.5)*V;

    %Energy grid
    E=[mu2-(10*kT)-(10*dE):dE:mu1+(10*kT)+(10*dE)];
        if V<0
            E=[mu1-(10*kT)-(10*dE):dE:mu2+(10*kT)+(10*dE)];
        end
        NE=size(E,2);[iV NE]
            f1=1./(1+exp((E-mu1)./kT));
            f2=1./(1+exp((E-mu2)./kT));

    %Initial guess
        n=zeros(1,NE);p=zeros(1,NE);
        sigin1=zeros(1,NE);sigout1=zeros(1,NE);
        sigin2=zeros(1,NE);sigout2=zeros(1,NE);
        sigin=0*ones(1,NE);sigout=0*ones(1,NE);
%Iterative solution of transport equation
change=1;it=1;
while change>1e-3
    for k=1:NE
    sig1=-i*gamma/2;gam1=i*(sig1-sig1');
    sig2=-i*gamma/2;gam2=i*(sig2-sig2');
        sigin1(k)=f1(k)*gam1;sigin2(k)=f2(k)*gam2;
        sigout1(k)=(1-f1(k))*gam1;sigout2(k)=(1-f2(k))*gam2;
        gamp=sigin(k)+sigout(k);
    G=inv((E(k)+zplus)-H0-U1-sig1-sig2+(i*0.5*gamp));
        A=i*(G-G');
            n(k)=real(G*((f1(k)*gam1)+(f2(k)*gam2)+sigin(k))*G');
            p(k)=A-n(k);
    end

    siginnew=D0*n;sigoutnew=D0*p;
    for iph=1:Nph
        inu=hnu(iph);
        if inu<NE
        ne=n([inu+1:NE]);ne=[ne zeros(1,inu)];
        na=n([1:NE-inu]);na=[zeros(1,inu) na];
        pe=p([inu+1:NE]);pe=[pe zeros(1,inu)];
        pa=p([1:NE-inu]);pa=[zeros(1,inu) pa];
            siginnew=siginnew+((Nhnu(iph)+1)*Dnu(iph)*ne)+(Nhnu(iph)*Dnu(iph)*na);
        sigoutnew=sigoutnew+(Nhnu(iph)*Dnu(iph)*pe)+((Nhnu(iph)+1)*Dnu(iph)*pa);
        end
    end

    change=sum(sum(abs(siginnew-sigin)));
    change=change+sum(sum(abs(sigoutnew-sigout)));
```

```
        sigin=((1-it)*sigin)+(it*siginnew);
        sigout=((1-it)*sigout)+(it*sigoutnew);
end

    I1=real((sigout1.*n)-(sigin1.*p));I1=sum(I1);
    I2=real((sigout2.*n)-(sigin2.*p));I2=sum(I2);
    I3=real((sigout.*n)-(sigin.*p));I3=sum(I3);

    I123=dE*[sum(I1) sum(I2) sum(I3)],%Normalized Conductance
    %IE=(dE/(V*V))*[sum(E.*I1) sum(E.*I2) sum(E.*I3)],%Normalized Power
    %kirchoff=[sum(I123) sum(IE)],%checking for conservation of current and energy current

II(iV)=sum(I2)*dE*I0;
end

G1=diff(II)./dV;VG=VV([2:NV]);
IETS=diff(G1)./dV;VETS=VV([3:NV]);

hold on
%h=plot(VV,II,'rx');
h=plot(VG,G1,'b–');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
%xlabel(' Voltage (V) --> ')
%ylabel(' d2I/dV2 --> ')
```

Appendix

% Fig.A.5.2, A.5.3

```
clear all

NE=1001;E=linspace(-.25,.25,NE);zplus=i*1e-3;dE=E(2)-E(1);kT=.00026;
Nep=5001;ep=linspace(-1,1,Nep);tau=0.05;dep=ep(2)-ep(1);delta=3.117*tau*tau/2
ep0=-25*delta;U=50*delta;[U/pi abs(ep0)]/delta
D=ones(1,Nep);f=1./(1+exp(ep./kT));fK=1./(1+exp(E./kT));tau=0.06;

for kE=1:NE
s0(kE)=dep*tau*tau*sum(D./(E(kE)-ep+zplus));
s1(kE)=dep*tau*tau*sum(D./(E(kE)-ep0-ep0-U+ep+zplus));
s2(kE)=dep*tau*tau*sum(D.*f./(E(kE)-ep+zplus));
s3(kE)=dep*tau*tau*sum(D.*f./(E(kE)-ep0-ep0-U+ep+zplus));
end

g=U./(E-ep0-U-s0-s0-s1);
GK=(1+(0.5*g))./(E-ep0-s0+(g.*(s2+s3)));
G=(1+(0.5*U./(E-ep0-U-s0)))./(E-ep0-s0);
A=i*(G-conj(G))/(2*pi);dE*sum(A)
AK=i*(GK-conj(GK))/(2*pi);dE*sum(AK)
dE*sum(AK.*fK)
del=-dE*sum(imag(s0))
```

```
hold on
%h=plot(E,-imag(s0));
%h=plot(E,imag(s1));
%h=plot(E,imag(s2),'mx');
%h=plot(E,imag(s3),'m');
h=plot(A,E,'b--');
h=plot(AK,E,'b');
set(h,'linewidth',[2.0])
set(gca,'Fontsize',[24])
grid on
xlabel(' D(E) per eV --> ')
ylabel(' E ( eV ) --> ')
```