NCN-Intel Summer School on

"Electronics from the Bottom-up"

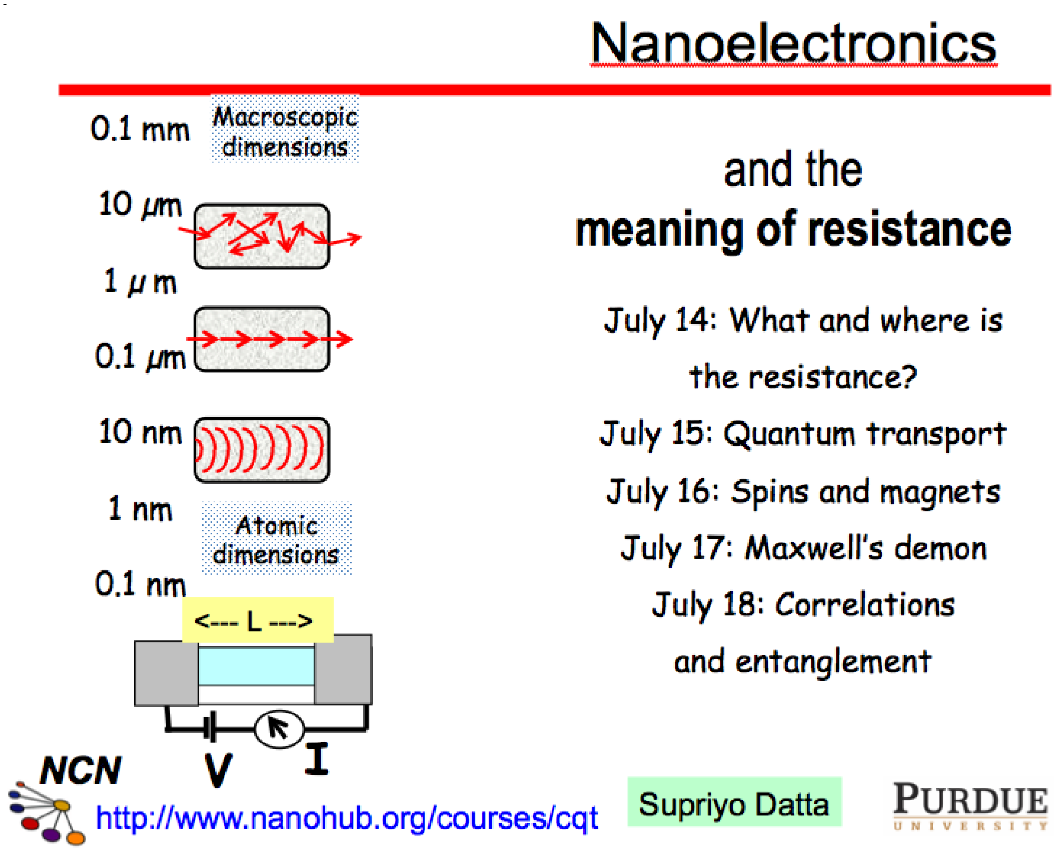
Purdue University, July 14-25, 2008

Nanoelectronics

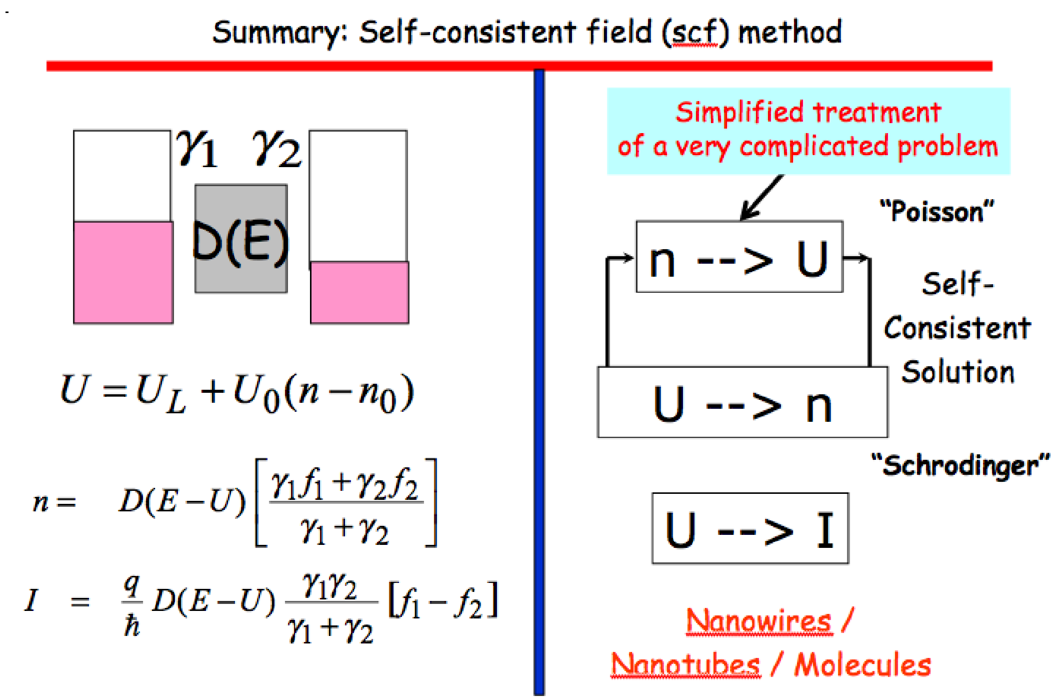
&the Meaning of Resistance

Supriyo Datta, datta@purdue.edu

July 14-18, 2008



July 14: What and where is the resistance?



Useful parameters: q = 1.6e-19 coul, h = 6.63e-34 joule-sec.

1. Calculate q^2/h, h/q^2.

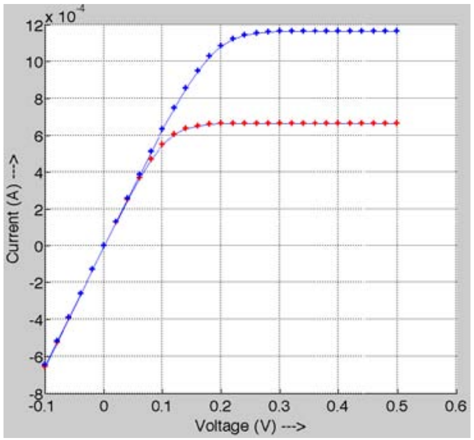
2. If γ = 1 meV, calculate γ/h, $q\gamma/h$

3. If electron density n_s = 1e-13/cm^2, calculate De Broglie wavelength for electron with energy equal to the Fermi energy. What is the corresponding contact resistance for a ballistic conductor.

%_1.1. Transistor: self-consistent I-V, simple code

```
% Calculating I-V charateristic
% Device structure
% |------------|--------------|------------|
% |Contact(T1) |   Channel    |Contact(T2) |
% |------------|--------------|------------|
%
clear all

%Parameters (all MKS, except energy which is in eV)
hbar=1.06e-34;  % Plank constant/(2*pi)
q=1.6e-19;      % Electron charge
m=0.2*9.1e-31;  % Electron effective mass
v=1e5;          % Surface recombination velocity
kT1=0.025;kT2=.025; % Temperature of the two contacts
L=1e-6;W=1e-6;      % Length and width of the channel
D=m*L*W/pi/hbar/hbar;   % Channel Density of states(2-D)
g1=hbar*v/L;g2=g1;      % Electron escape rates at the contacts
kT=(kT1+kT2)/2;Ef=0.1;dE=0.001;E=[0:dE:1];
f0=1./(1+exp((E-Ef)./kT));
N0=sum(q*dE*D*f0);
U0=0e-1/N0;     % Electron charging energy

% Following calculates both currents and energy current at each bias point

%Bias
ii=1;dV=0.02;
for V=0:dV:0.5
UL=1e-12;
change=100;U=UL;
while change>1e-6 % Sef-consistent loop between charge and potential
mu1=Ef-U;mu2=Ef-U-V;
f1=1./(1+exp((E-mu1)./kT1));    % Fermi funciton at the contact 1
f2=1./(1+exp((E-mu2)./kT2));    % Fermi funciton at the contact 2
f=(g1*f1+g2*f2)./(g1+g2);       % Electron distribution in the channel
  N=sum(q*dE*D*f);              % Electron number in the channel
  Unew=UL+U0*(N-N0);
change=sum(abs(U-Unew))/sum(abs(U+Unew));
   U=U+0.1*(Unew-U);            % Channel potential
end

curr1(ii)=(q*q*D*dE/hbar)*sum(g1*(f1-f));   % Current at the conatct 1 junction
ecurr1(ii)=(q*q*D*dE/hbar)*sum(g1*(f1-f).*(E-mu1)); % Heat current at the contact 1
junction
curr2(ii)=(q*q*D*dE/hbar)*sum(g2*(f-f2));   % Current at the conatct 2 junction
ecurr2(ii)=(q*q*D*dE/hbar)*sum(g2*(f-f2).*(E-mu2)); % Heat current at the contact 2
juction
volt(ii)=V;ii=ii+1;
end
```

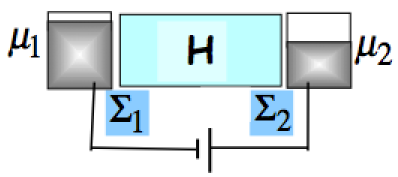
```
figure(1)
hold on
h=plot(volt,curr1,'b');h=plot(volt,curr2,'ro');
```



→U0 = 0

Day 2: Quantum transport

Coherent transport



•Semi-empirical
•First principles

$\Gamma = i[\Sigma - \Sigma^+]$

Green function $$[G] = [EI - H - \Sigma_1 - \Sigma_2]^{-1}$$

"Density of states" $$A = i[G - G^+]$$

"Electron density"

$\varepsilon \rightarrow [H]$

$\gamma \rightarrow [\Gamma], [\Sigma]$

$$G^n = G \overbrace{\Sigma_1^{in}}^{[\Gamma_1] f_1} G^+ + G \overbrace{\Sigma_2^{in}}^{[\Gamma_2] f_2} G^+$$

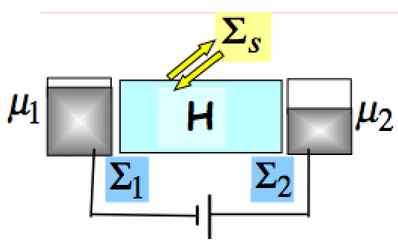
$n \rightarrow [\rho]$

$n(E) \rightarrow [G^n(E)]$

$D(E) \rightarrow [A(E)]$

Current $$\frac{I_1}{q/\hbar} = Trace\left([\overbrace{\Sigma_1^{in}}^{[\Gamma_1] f_1} A] - [\Gamma_1 G^n] \right)$$

Incoherent transport



Green function $$[G] = [EI - H - \Sigma_1 - \Sigma_2 - \Sigma_s]^{-1}$$

"Density of states" $$A = i[G - G^+]$$

"Electron density"

$\Gamma = i[\Sigma - \Sigma^+]$

$$G^n = G\Gamma_2 G^+ f_2 + G\Gamma_1 G^+ f_1 + G\Sigma_s^{in} G^+$$

$\varepsilon \rightarrow [H]$

$\gamma \rightarrow [\Gamma], [\Sigma]$

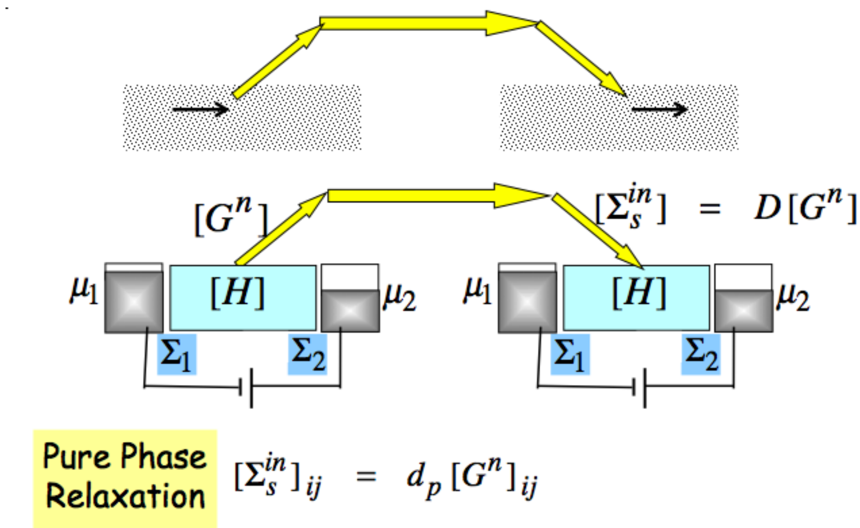
Current $$\frac{I_1}{q/\hbar} = Trace\left([\Gamma_1 A] f_1 - [\Gamma_1 G^n] \right)$$

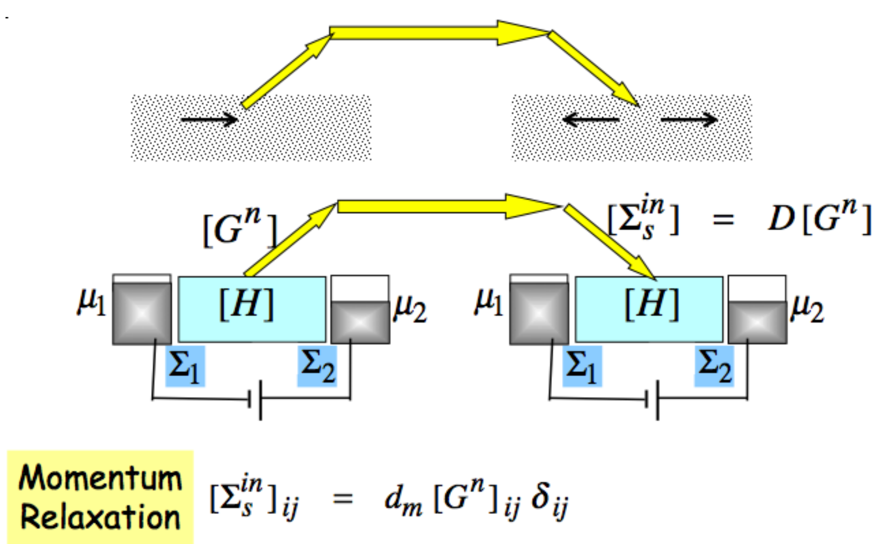
$n \rightarrow [\rho]$

Dephasing model: $$[\Sigma_s^{in}] = D[G^n]$$

$n(E) \rightarrow [G^n(E)]$

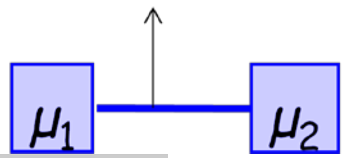
$D(E) \rightarrow [A(E)]$

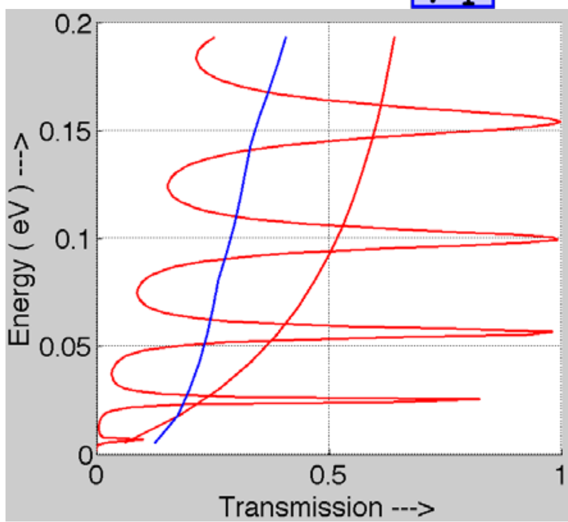

$[G^n]$
$[\Sigma_s^{in}] = D[G^n]$
μ_1
$[H]$
μ_2
Σ_1
Σ_2
Pure Phase Relaxation
$[\Sigma_s^{in}]_{ij} = d_p [G^n]_{ij}$


$[G^n]$
$[\Sigma_s^{in}] = D[G^n]$
μ_1
$[H]$
μ_2
Σ_1
Σ_2
Momentum Relaxation
$[\Sigma_s^{in}]_{ij} = d_m [G^n]_{ij} \delta_{ij}$

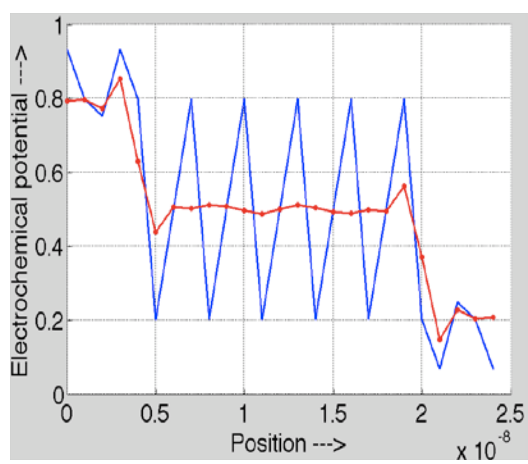
%_2.1. NEGF code, 1D

```
%. 1D with  pure phase relaxation
clear all
%Parameters (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;m=0.2*9.1e-31;a=1e-9;t0=(hbar^2)/(2*m*(a^2)*q);

% Device structure
Np=25;N1=5;N2=21;X=a*[0:1:Np-1];
L=diag([1 zeros(1,Np-1)]);R=diag([zeros(1,Np-1) 1]);
D=1e-2;sigB=zeros(Np);siginB=zeros(Np);

% Hamiltonian set-up
H0=2*t0*diag(ones(1,Np))-t0*diag(ones(1,Np-1),1)-t0*diag(ones(1,Np-1),-1);
UB1=1*0.25;UB2=1*0.25;H0(N1,N1)=H0(N1,N1)+UB1;H0(N2,N2)=H0(N2,N2)+UB2;
H=H0;

ii=1;dE=0.00125;zplus=i*1e-12;
for EE=0.001:dE:t0
%for EE=t0:-dE:t0
   ck=(1-(EE+zplus)/(2*t0));ka=acos(ck);s1=-t0*exp(i*ka);s2=-t0*exp(i*ka);
sig1=kron(L,s1);sig2=kron(R,s2);    % contact self energy
gam1=i*(sig1-sig1');gam2=i*(sig2-sig2');

change=100;
while change>1e-6 % calculating G self-consistently
        G=inv((EE*eye(Np))-H-sig1-sig2-sigB);
sigBnew=D*G;
change=(sum(sum(abs(sigBnew-sigB))))/(sum(sum(abs(sigBnew+sigB))));
sigB=sigB+0.25*(sigBnew-sigB);
end
   A=real(diag(i*(G-G')));change=100;ii
while change>1e-6 % calculating Gn self-consistently
Gn=G*(gam1+siginB)*G';
siginBnew=D*Gn;
change=(sum(sum(abs(siginBnew-siginB))))/(sum(sum(abs(siginBnew+siginB))));
siginB=siginB+0.25*(siginBnew-siginB);
end

Tcoh(ii)=real(trace(gam1*G*gam2*G'));
TM(ii)=real(trace(gam2*Gn));
mu(:,ii)=real(diag(Gn))./A;E(ii)=EE;ii=ii+1;
end
%%
hold on
figure(1)
h=plot(TM,E,'r');
figure(2)
h=plot(X,mu(:,1),'ro');
```


μ_1
μ_2


Energy (eV) --->
Transmission --->
0.2
0.15
0.1
0.05
0
0
0.5
1


μ_1
μ_2

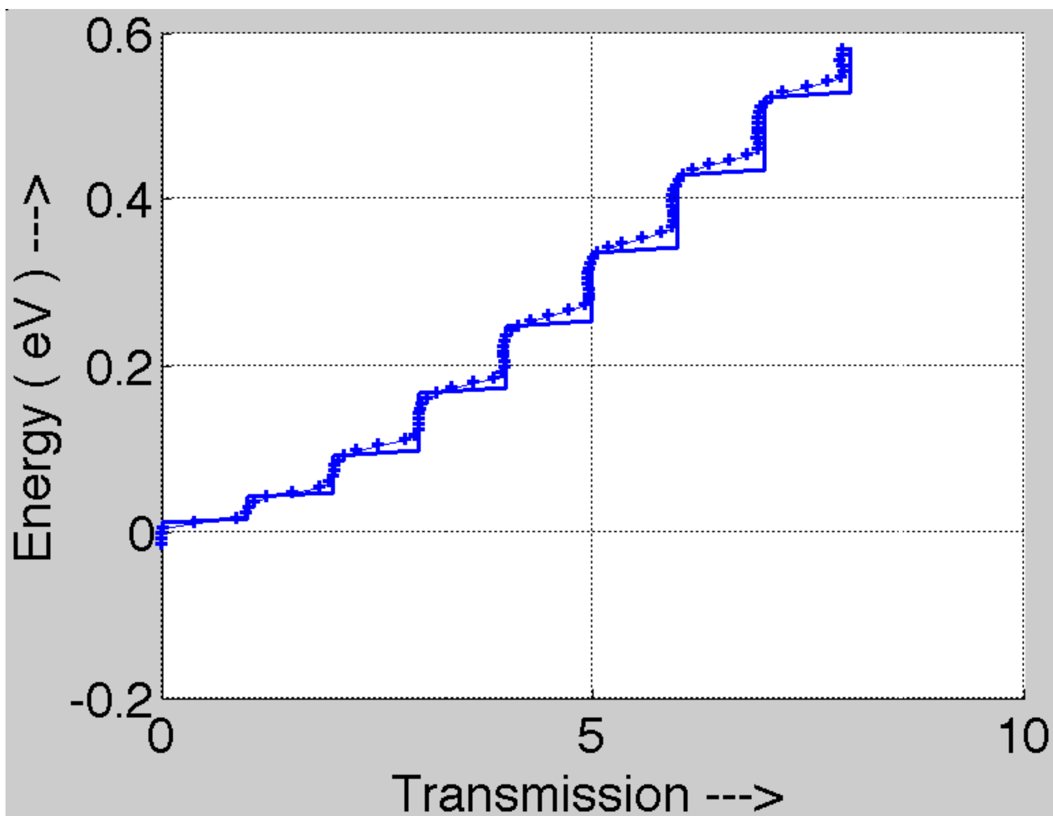

Electrochemical potential --->
Position --->
x 10^-8
1
0.8
0.6
0.4
0.2
0
0
0.5
1
1.5
2
2.5

% 2.2. NEGF code, 2D

```
% 2-D NEGF with Wide-Narrow-Wide structure
clear all
hbar=1.06e-34;q=1.6e-19;m=0.2*9.1e-31;a=1e-9;t0=(hbar^2)/(2*m*(a^2)*q);

NN=12;bn=-t0*eye(NN);b=-t0*diag(1,NN-1)';
an=4*t0*diag(ones(1,NN))-t0*diag(ones(1,NN-1),1)-t0*diag(ones(1,NN-1),-1); %
narrow region

% an  b  0 |       |
% b' an  b | bn    |
% 0  b' an | 0     |
%---------- ------- -------
%    bn' 0 | an bn |
%          | bn'an | 0 bn'
%---------- ------- -------
%          |    0  | an b  0
%          |   bn  | b' an b
%          |       | 0  b' an

w=2;Nw=1+2*w;   % width of wide region in units of narrow region (an)
Np=5;           % # of slices in narrow region
NT=Np+Nw+Nw;
HD=kron(eye(Np+2*Nw),an); % set-up diagonal blocks
HD1a=kron(diag([ones(1,Nw-1) zeros(1,Np+1) ones(1,Nw-1)],1),b); % set-up upper
diagonal blocks in wide region
HD1b=kron(diag([zeros(1,Nw) ones(1,Np-1) zeros(1,Nw)],1),bn);   % set-up upper
diagonal blocks in narrow region
hd2=zeros(NT);hd2(w+1,Nw+1)=1;hd2(NT-w,NT-Nw)=1;HD2=kron(hd2,bn); % set-up
coupling between wide and narrow region
H=HD+HD1a+HD1b+HD2+HD1a'+HD1b'+HD2'; % complete Hamiltonian

HC=kron(eye(Nw),an)+kron(diag(ones(1,Nw-1),1),b)+kron(diag(ones(1,Nw-1),-1),b');
[VC,DC]=eig(HC);DC=diag(DC);
dE=0.00625;zplus=i*1e-12;
D=1e-3;sigB=zeros(NT*NN);siginB=zeros(NT*NN);ctr=0;

ii=1; for EE=3*t0:-dE:-0.1*t0
% for EE=t0:-dE:t0
   ck=(DC-EE-zplus)./(2*t0);ka=acos(ck);
s=VC*diag(-t0*exp(i*ka))*VC'; % contact self energy in wide region
sig1=[s zeros(Nw*NN,(Np+Nw)*NN);zeros((Np+Nw)*NN,NT*NN)];
sig2=[zeros((Np+Nw)*NN,NT*NN);zeros(Nw*NN,(Np+Nw)*NN) s];
gam1=i*(sig1-sig1');gam2=i*(sig2-sig2');

change=100;
while change>1e-6 % calculating G self-consistently
      G=inv((EE*eye(NT*NN))-H-sig1-sig2-sigB);
sigBnew=D*G;
change=ctr*(sum(sum(abs(sigBnew-sigB))))/(sum(sum(abs(sigBnew+sigB))));
sigB=sigB+ctr*(sigBnew-sigB);
```



```
end
   A=real(diag(i*(G-G')));change=100;ii
while change>1e-6 % calculating Gn self-consistently
Gn=G*(gam1+siginB)*G';
siginBnew=D*Gn;
change=ctr*(sum(sum(abs(siginBnew-siginB))))/(sum(sum(abs(siginBnew+siginB))));
siginB=siginB+ctr*(siginBnew-siginB);
end

Tcoh(ii)=real(trace(gam1*G*gam2*G'));TM(ii)=real(trace(gam2*Gn));
E(ii)=EE;ii=ii+1;
end
%%
hold on
figure(1)
h=plot(TM,E,'b+');
```

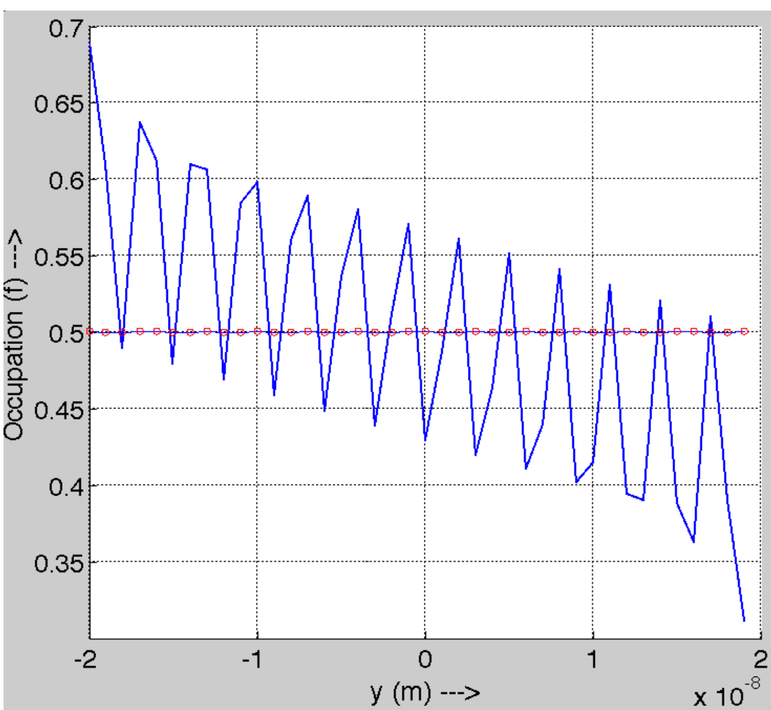


% 2.3. NEGF2D with B-field

```
%%% 2-D with magnetic field
% B-field: A_x = By
clear all

% Inputs
hbar=1.06e-34;q=1.6e-19;m=0.2*9.1e-31;a=1e-9;B=1;
t0=(hbar^2)/(2*m*(a^2)*q);

NW=40;Np=2;L=zeros(Np);R=L;L(1,1)=1;R(Np,Np)=1;
Y=a*([0:1:NW-1]-0.5*NW);
HW=eye(NW);
if NW==1
HW(1,1)=0.5;
end

al=4*t0;by=-t0;
alpha=kron(HW,al);
if NW>1
alpha=alpha+kron(diag(ones(1,NW-1),+1),by)+kron(diag(ones(1,NW-1),-1),by');
end
beta=-t0*diag(exp(i*q*B*a*Y/hbar)); % magnetic field
H=kron(eye(Np),alpha)+kron(diag(ones(1,Np-1),+1),beta)+kron(diag(ones(1,Np-1),-
1),beta');

D=4e-2;ctr=0;sigB=zeros(Np*NW);siginB=zeros(Np*NW);
ii=1;zplus=i*1e-12;dE=0.005;
for EE=t0:-dE:0

galpha=(EE+zplus)*eye(NW)-alpha;
if ii==1 % initialization
g1=galpha;g2=galpha;
end

change=1;
while change >5e-4 % calculating source contact self energy
        Gs=inv(galpha-beta'*g1*beta);
change=sum(sum(abs(Gs-g1)))/(sum(sum(abs(g1)+abs(Gs))));
g1=0.95*Gs+0.05*g1;
end
sig1=beta'*g1*beta;sig1=kron(L,sig1);gam1=i*(sig1-sig1');

change=1;
while change >5e-4 % calculating drain contact self energy
        Gs=inv(galpha-beta*g2*beta');
change=sum(sum(abs(Gs-g2)))/(sum(sum(abs(g2)+abs(Gs))));
g2=0.95*Gs+0.05*g2;
end
sig2=beta*g2*beta';sig2=kron(R,sig2);gam2=i*(sig2-sig2');

change=1;
```



```
while change>5e-5 % calculating G self-consistently
        G=inv((EE*eye(Np*NW))-H-sig1-sig2-sigB);
sigBnew=D*G;
change=ctr*(sum(sum(abs(sigBnew-sigB))))/(sum(sum(abs(sigBnew+sigB))));
sigB=sigB+0.25*ctr*(sigBnew-sigB);
end
    A=i*(G-G');change=1;
while change>5e-5 % calculating Gn self-consistently
Gn=G*(gam1+siginB)*G';
siginBnew=D*Gn;
change=ctr*(sum(sum(abs(siginBnew-siginB))))/(sum(sum(abs(siginBnew+siginB))));
siginB=siginB+0.25*ctr*(siginBnew-siginB);
end

TM1(ii)=real(trace(gam1*(A-Gn)));
TM2(ii)=real(trace(gam2*Gn));
n(:,ii)=real(diag(Gn));DD(:,ii)=real(diag(A));mu=n./DD;E(ii)=EE;ii
ii=ii+1;
end
%%
hold on
figure(1)
h=plot(TM2,E,'r');
figure(2)
h=plot(Y,mu([1:1:NW],1),'b');
```



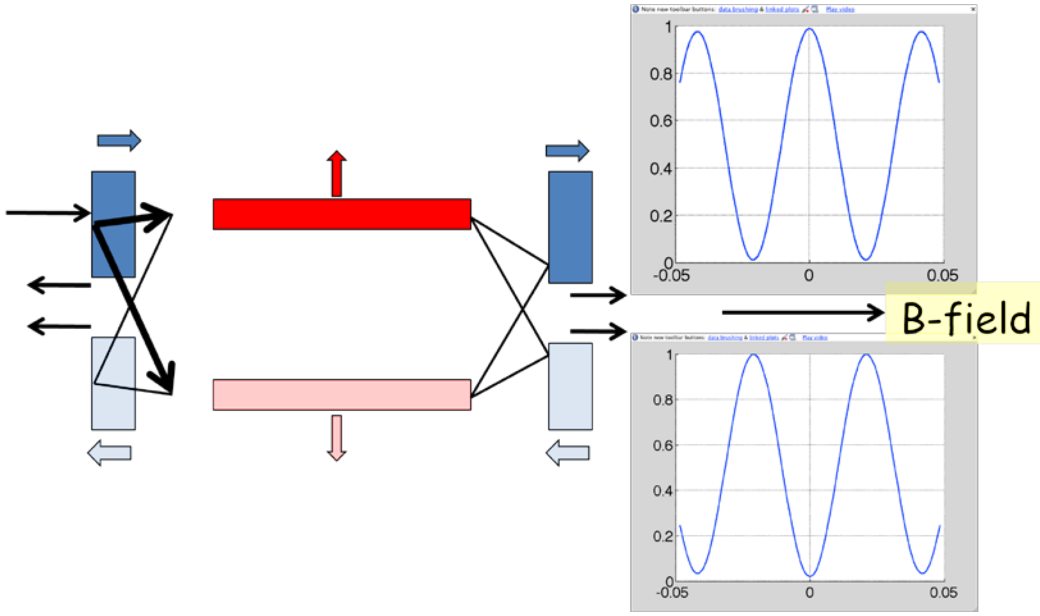
Day 3: Spins and magnets

% 3.1.Spin-NEGF code, 1D

```
clear all
tic

%---------Pauli Spin matrices----------%
sx=[0 1; 1 0];
sy=[0 -i; i 0];
sz=[1 0; 0 -1];

%constants (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;m=0.2*9.1e-31;

%polarization of the contacts
Pc=0.99;

theta1=pi/2;theta2=pi/2;

Utrans_L=[cos(theta1/2) -sin(theta1/2);sin(theta1/2) cos(theta1/2)];%Unitary
Transformation matrix for Left Contact
Utrans_R=[cos(theta2/2) -sin(theta2/2);sin(theta2/2) cos(theta2/2)];%Unitary
Transformation matrix for Right Contact

%inputs
a=1e-9;
t0=(hbar^2)/(2*m*(a^2)*q);
Np=25;N1=5;N2=21; % N1, N2 positions of scatter is any
X=a*[0:1:Np-1];
L=diag([1 zeros(1,Np-1)]);R=diag([zeros(1,Np-1) 1]);
NC=13;C=diag([zeros(1,NC-3),ones(1,5),zeros(1,Np-NC-2)]);

D=1e-20;%Scattering Strength
sigB=zeros(2*Np);%Self Energy due to scattering
siginB=zeros(2*Np);
%-----------------------------Hamiltonian Matrix-------------------------%
H0=2*t0*diag(ones(1,Np))-t0*diag(ones(1,Np-1),1)-t0*diag(ones(1,Np-1),-1);
UBup=0*10;UBdn=0*10; %Magnetic Barrier

ii=1;dE=0.00125;zplus=i*1e-12;

for EE=t0:-dE:t0
  jj=1;

  for HB=-0.25*t0:0.00625*t0:+0.25*t0  %External magnetic Field HB
    H=kron(H0,eye(2))+kron(eye(Np),[HB 0;0 -HB])+kron(C,[UBup 0;0 UBdn]);
    ck=(1-(EE+zplus)/(2*t0));ka=acos(ck);
    su=-t0*exp(i*ka)*0.5*(eye(2)+Pc*sz);
    sd=-t0*exp(i*ka)*0.5*(eye(2)-Pc*sz);
    sig1u=kron(L,Utrans_L*su*Utrans_L');%Self Energy Matrix for Left Up-Spin
Contact
```



```
    sig1d=kron(L,Utrans_L*sd*Utrans_L');%Self Energy Matrix for Left dn-Spin
Contact
    sig2u=kron(R,Utrans_R*su*Utrans_R');%Self Energy Matrix for Right Up-Spin
Contact
    sig2d=kron(R,Utrans_R*sd*Utrans_R');%Self Energy Matrix for Right dn-Spin
Contact
    gam1u=i*(sig1u-sig1u');gam1d=i*(sig1d-sig1d');
    gam2u=i*(sig2u-sig2u');gam2d=i*(sig2d-sig2d');

    change=100;
    while change>1e-6
      %---------------Calculation of Green's function,G self-consistently--------------%
      G=inv((EE*eye(2*Np))-H-sig1u-sig1d-sig2u-sig2d-sigB);
      sigBnew=D*G;
      change=(sum(sum(abs(sigBnew-sigB))))/(sum(sum(abs(sigBnew+sigB))));
      sigB=sigB+0.25*(sigBnew-sigB);

    end

    A=i*(G-G');%Evaluating Broadening function, A
    change=100;jj

    while change>1e-6
      Gn=G*(gam1u+siginB)*G';
      siginBnew=D*Gn;
      change=(sum(sum(abs(siginBnew-
siginB))))/(sum(sum(abs(siginBnew+siginB))));
      siginB=siginB+0.25*(siginBnew-siginB);
    end

    TM1d(jj)=real(trace(gam1d*Gn));TM2u(jj)=real(trace(gam2u*Gn));
    TM2d(jj)=real(trace(gam2d*Gn));TM1u(jj)=real(trace(gam1u*(A-Gn)));
    B(jj)=HB;jj=jj+1;
  end
end


hold on
h=plot(B,TM1d,'b');
hold on
figure
h=plot(B,TM1u,'b');
hold on
figure
h=plot(B,TM2d,'b');
hold on
figure
h=plot(B,TM2u,'b');
toc
```


B-field
1
0.8
0.6
0.4
0.2
0
-0.05
0
0.05

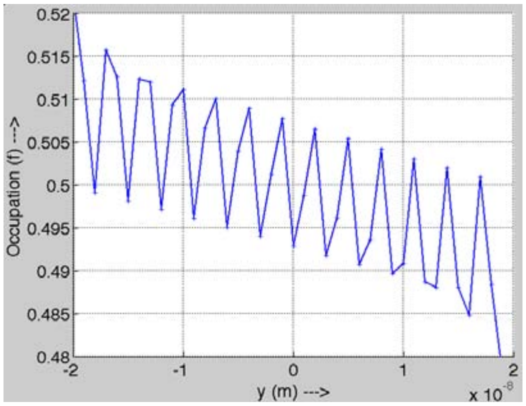
% 3.2. Spin-NEGF code, 2D

```
% Rashba term: sx*ky-sy*kx = (1/2/i/a) (e*ikya-e*-ikya)*sx-(e*ikxa-e*-ikxa)*sy
% B-field: A_x = By
clear all
tic

%---------Pauli Spin matrices----------%
sx=[0 1; 1 0];
sy=[0 -i; i 0];
sz=[1 0; 0 -1];

%constants (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;m=0.2*9.1e-31;
rashba=0e-12;
B=10;

%inputs
a=1e-9;
t0=(hbar^2)/(2*m*(a^2)*q);
NW=40; %Number of points along transverse direction
Np=2; %Number of points along longitudinal direction
L=zeros(Np);R=L;L(1,1)=1;R(Np,Np)=1;
Y=a*([0:1:NW-1]-0.5*NW);

%-----------------------------Hamiltonian Matrix-------------------------%
HW=eye(NW);
if NW==1
    HW(1,1)=0.5;
end

al=4*t0*eye(2);
by=-t0*eye(2)+(rashba/i/2/a)*sx;bx=-(rashba/i/2/a)*sy;%adding Rashba terms to
Hamiltonian
alpha=kron(HW,al);
if NW>1
alpha=alpha+kron(diag(ones(1,NW-1),+1),by)+kron(diag(ones(1,NW-1),-1),by');
end
beta=kron(eye(NW),bx)+kron(-t0*diag(exp(i*q*B*a*Y/hbar)),eye(2));
H=kron(eye(Np),alpha)+kron(diag(ones(1,Np-1),+1),beta)+kron(diag(ones(1,Np-1),-
1),beta');

D=4e-2;%Scattering Strength
ctr=0;
sigB=zeros(2*Np*NW);
siginB=zeros(2*Np*NW);%Self Energy due to scattering
ii=1;zplus=i*1e-12;dE=0.005;

for EE=t0:-dE:t0
    galpha=(EE+zplus)*eye(2*NW)-alpha;
    if ii==1
    g1=galpha;g2=galpha;
```

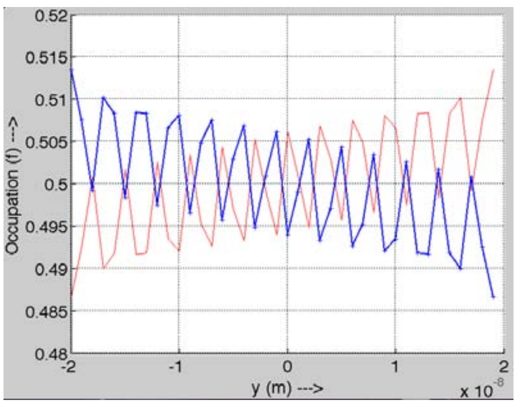
```
   end

   change=1;
   while change >5e-4
      Gs=inv(galpha-beta'*g1*beta);%Evaluating Surface Green's Function, Gs for left
contact
      change=sum(sum(abs(Gs-g1)))/(sum(sum(abs(g1)+abs(Gs))));
      g1=0.95*Gs+0.05*g1;
   end
   sig1=beta'*g1*beta;
   sig1=kron(L,sig1);%Self Energy Matrix for Left Contact
   gam1=i*(sig1-sig1');

   change=1;
   while change >5e-4
      Gs=inv(galpha-beta*g2*beta');%Evaluating Surface Green's Function, Gs for right
contact
      change=sum(sum(abs(Gs-g2)))/(sum(sum(abs(g2)+abs(Gs))));
      g2=0.95*Gs+0.05*g2;
   end
   sig2=beta*g2*beta';
   sig2=kron(R,sig2);%Self Energy Matrix for Right Contact
   gam2=i*(sig2-sig2');

   change=1;
   while change>5e-5
      G=inv((EE*eye(2*Np*NW))-H-sig1-sig2-sigB);%Calculation of Green's function,G
self-consistently
      sigBnew=D*G;
      change=ctr*(sum(sum(abs(sigBnew-sigB))))/(sum(sum(abs(sigBnew+sigB))));
      sigB=sigB+0.25*ctr*(sigBnew-sigB);
   end
   A=i*(G-G');change=1;

   while change>5e-5
      Gn=G*(gam1+siginB)*G';
      siginBnew=D*Gn;
      change=ctr*(sum(sum(abs(siginBnew-
siginB))))/(sum(sum(abs(siginBnew+siginB))));
      siginB=siginB+0.25*ctr*(siginBnew-siginB);
   end

   TM1(ii)=real(trace(gam1*(A-Gn)));
   TM2(ii)=real(trace(gam2*Gn));
   n(:,ii)=real(diag(Gn));%Electron Density
   DD(:,ii)=real(diag(A));%Density of States
   mu=n./DD;E(ii)=EE;ii
   ii=ii+1;

end
```

```
hold on
% h=plot(TM2,E,'b');
% hold on
figure
h=plot(Y,mu([2:2:2*NW],1),'b');
hold on
figure
h=plot(Y,mu([1:2:2*NW],1),'r');
toc
```

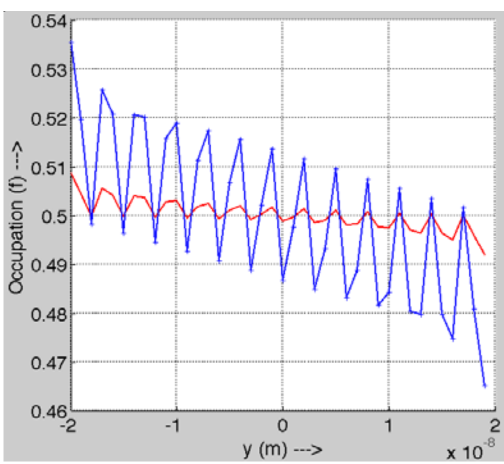
$B = 1\,T, \alpha = 0$



$B = 0\,T, \alpha = 1e-11\,eV-m$



$B = 1\,T, \alpha = 1e-11\,eV-m$



Day 4: Maxwell's demon

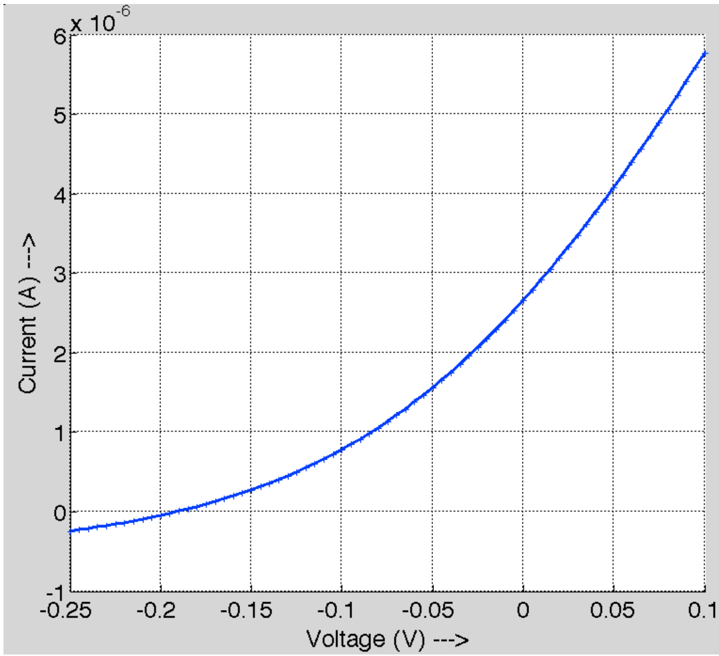
% 4.1. Seebeck and Peltier coefficients, simple code

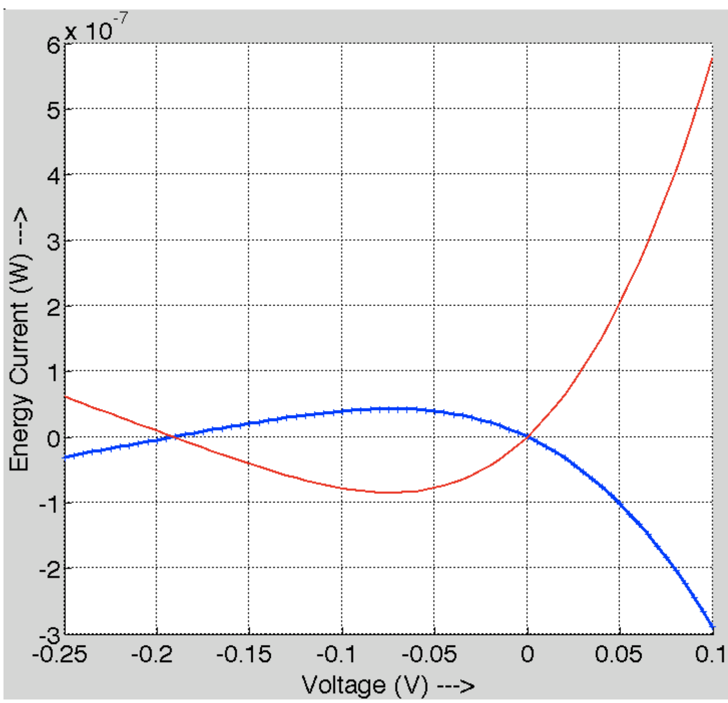
```
%%% Thermoelectric Effect %%%
% Finding Seebeck and Peltier coeefficient
% Device structure
% |------------|--------------|------------|
% |Hot         |              |Cold        |
% |Contact(T1) | Channel      |Contact(T2) |
% |------------|--------------|------------|
%
% Density of states used : 2-D
% Seebeck coefficient = (Voc)./(T1-T2)
%        Voc = open circuit voltage,
%        T1-T2 = temperature difference,
% Peltier Coefficient at hot or cold junctions
%        = Heat flux./current
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
clear all;
clc;
warning off;

%Parameters
hbar=1.06e-34;   %Plancks constant/(2*pi)
q=1.6e-19;       %Electron charge
m=0.2*9.1e-31;   %Electron effective mass
v=1e5;           %Surface recombination velocity

kT1=0.026;kT2=kT1*299/300; %Temperature of the two contacts
L=1e-8;W=1e-6;   % Length and width of the channel
D=m*L*W/pi/hbar/hbar; % Channel Density-of-states
Ef=0;              % Fermi level of the device
g1=hbar*v/L;        % electron escape rates at the contacts
g2=g1;
kT=(kT1+kT2)/2;

%Energy Grid
dE=1e-5;
E=[0.029:dE:0.031]; %E=[0:dE:0.25];

%Bias Grids
ii=1;dV=1e-5;

% Following loop calculates both currents and
% energy currents at the two contacts for
% each bias point

for V=-2e-4:dV:2e-4
```

```
mu1=Ef+V/2;mu2=Ef-V/2;       % Contact Fermi levels
f1=1./(1+exp((E-mu1)./kT1));  % Fermi funciton at hot(left)
f2=1./(1+exp((E-mu2)./kT2));  % Fermi funciton at cold(right)
f=(g1*f1+g2*f2)./(g1+g2);     % Electron distribution in the channel
curr1(ii)=(q*q*D*dE/hbar)*sum(g1*(f1-f)); % Current at the hot junction
ecurr1(ii)=(q*q*D*dE/hbar)*sum(g1*(f1-f).*(E-mu1)); % Heat flux at the hot junction
curr2(ii)=(q*q*D*dE/hbar)*sum(g1*(f-f2)); % Current at the cold junction
ecurr2(ii)=(q*q*D*dE/hbar)*sum(g1*(f-f2).*(E-mu2)); % Heat flux at the cold junction
volt(ii)=V;ii=ii+1;
end

figure(1);
hold on
h=plot(volt,curr1,'bo');
h=plot(volt,curr2,'b');
set(h,'linewidth',[3.0])
set(gca,'Fontsize',[24])
xlabel(' Voltage (V) ---> ');
ylabel(' Current (A) ---> ');
grid on

figure(2);
hold on
h=plot(volt,ecurr1,'bo');
h=plot(volt,ecurr2,'b');
set(h,'linewidth',[3.0])
set(gca,'Fontsize',[24])
xlabel(' Voltage (V) ---> ');
ylabel(' Energy Currents (W) ---> ');

figure(3);
hold on
h=plot(volt,ecurr1./curr1,'bo');
h=plot(volt,ecurr2./curr2,'b');
set(h,'linewidth',[3.0])
set(gca,'Fontsize',[24])
xlabel(' Voltage (V) ---> ');
ylabel(' Peltier coefficient (W/A)---> ');
```

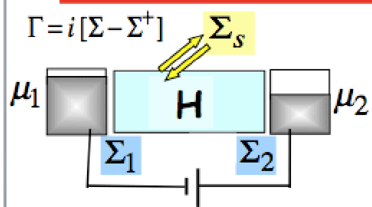
The following code assumes elastic interactions with scatterers NOT in equilibrium.

```
% 4.2. Simple code with elastic scattering
clear all

%Parameters
kT=0.025*2;% Temperature of contacts, Fig.9,10
gg=4e-5*2;% Conductance of each junction = device conductance*2
Pc=0.99;Pa=0;% Contact polarization, Asymmetry
  g1a=gg*(1+Pc)*(1+Pa);g1b=gg*(1-Pc)*(1+Pa);
  g2a=gg*(1+Pc)*(1-Pa);g2b=gg*(1-Pc)*(1-Pa);
k=1;g1u=g1a;g1d=g1b;if k==1
  g2u=g2b;g2d=g2a;%Antiparallel
  end;if k==2
  g2u=g2a;g2d=g2b;%Parallel
  end
g=gg*1;% Spin-flip conductance
Fu=0;Fd=1-Fu;dE=0.005;E=[-0.25:dE:0.25];

ii=1;for V=-0.2:dE:0.1
% for V=0.05:0.2*kT:0.05
mu1=(0.5)*V;mu2=(-0.5)*V;
  f1d=1./(1+exp((E-mu1)./kT));f1u=f1d;
    f2d=1./(1+exp((E-mu2)./kT));f2u=f2d;
      fu=f1u;fd=f2d;%Initial guess

  change=1;while change>1e-10
    Su=(g1u*f1u)+(g2u*f2u)+(g*fd.*(1-fu).*Fu)-(g*fu.*(1-fd).*Fd);
    Sd=(g1d*f1d)+(g2d*f2d)+(g*fu.*(1-fd).*Fd)-(g*fd.*(1-fu).*Fu);
      fup=Su./(g1u+g2u);fdn=Sd./(g1d+g2d);
        change=sum(abs(fup-fu)+abs(fdn-fd));
    fu=fu+(0.05*(fup-fu));fd=fd+(0.05*(fdn-fd));end

  %Sum over energy
      I1(ii)=(dE*sum((g1u*(f1u-fu))+(g1d*(f1d-fd))));
      I2(ii)=dE*sum((g2u*(fu-f2u))+(g2d*(fd-f2d)));
      IE1(ii)=dE*sum((E-mu1).*((g1u*(f1u-fu))+(g1d*(f1d-fd))));
      IE2(ii)=dE*sum((mu2-E).*((g2u*(fu-f2u))+(g2d*(fd-f2d))));
      Idu(ii)=dE*g*sum(fd.*(1-fu));Iud(ii)=dE*g*sum(fu.*(1-fd));
      volt(ii)=V;ii=ii+1;
end

hold on
h=plot(volt,IE1,'b');
h=plot(volt,IE2,'b+');
%h=plot(volt,volt.*I1,'r');
```


x 10^-6
Current (A) --->
Voltage (V) --->
6
5
4
3
2
1
0
-1
-0.25
-0.2
-0.15
-0.1
-0.05
0
0.05
0.1


x 10^-7
Energy Current (W) --->
Voltage (V) --->
6
5
4
3
2
1
0
-1
-2
-3
-0.25
-0.2
-0.15
-0.1
-0.05
0
0.05
0.1

NEGF equations .. including "everything" .. almost ..



Green function

$$[G] = [EI - H - \Sigma_1 - \Sigma_2 - \Sigma_s]^{-1}$$

"Electron density"

$$G^n = G\Gamma_2 G^+ f_2 + G\Gamma_1 G^+ f_1 + G\Sigma_s^{in} G^+$$

"Hole density"

$$G^p = G\Gamma_2 G^+ (1 - f_2) + G\Gamma_1 G^+ (1 - f_1) + G\Sigma_s^{out} G^+$$

"Density of states"

$$A = G^n + G^p = i[G - G^+]$$

Broadening

$$[\Gamma_s] = [\Sigma_s^{in} + \Sigma_s^{out}] = i[\Sigma_s - \Sigma_s^+]$$

Dephasing

$$[\Sigma_s^{in}(E)] = [[D(\varepsilon)]]\,[G^n(E - \varepsilon)]$$

$$[\Sigma_s^{out}(E)] = [[D(-\varepsilon)]]^T\,[G^p(E - \varepsilon)]$$

$$[\Sigma_s(E)] = [h(E)] - \frac{i}{2}[\Gamma_s(E)]$$

NCN http://www.nanohub.org/courses/cqt

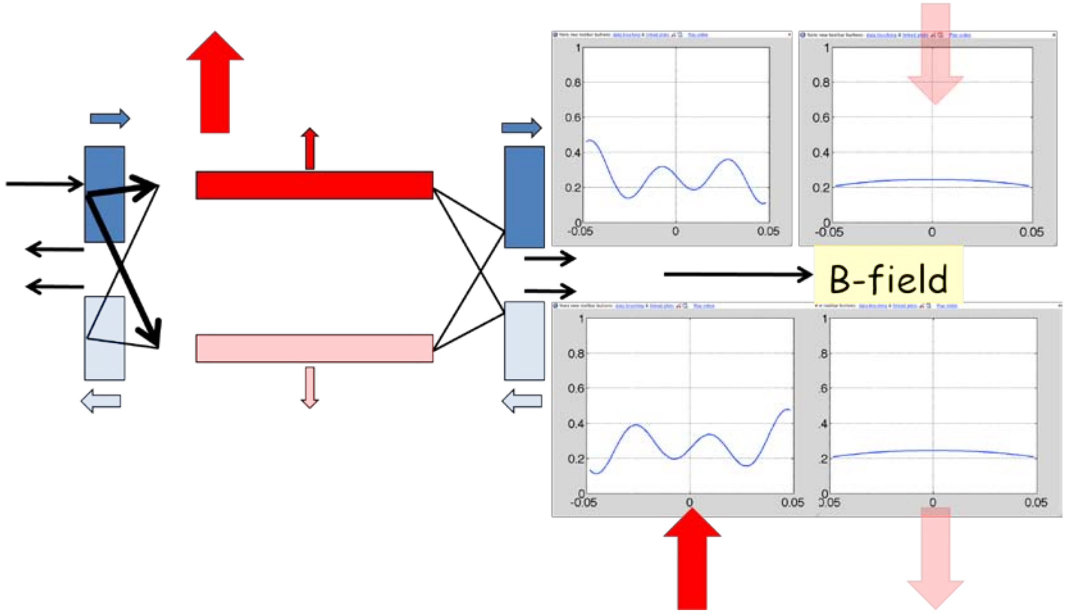
Supriyo Datta

Purdue University

Day 5: Correlations and entanglement

```
% 5.1.Entangled spin-NEGF code, 1D
clear all
%Constants
hbar=1.06e-34;q=1.6e-19;m=0.2*9.1e-31;a=1e-9;t0=(hbar^2)/(2*m*(a^2)*q);
sx=[0 1;1 0];sy=[0 -i;i 0];sz=[1 0;0 -1];          % Pauli Spin Matrices
thet1=1*pi/2;thet2=1*pi/2;Pc=0.99;                % Contact Polarization
U1=[cos(thet1/2) -sin(thet1/2);sin(thet1/2) cos(thet1/2)]; % Transformation Matrix
U2=[cos(thet2/2) -sin(thet2/2);sin(thet2/2) cos(thet2/2)]; % Transformation Matrix

Np=25;N1=5;N2=21;X=a*[0:1:Np-1];                      % N1, N2 position of scatterer if
any
NC=13;C=diag([zeros(1,NC-3),ones(1,5),zeros(1,Np-NC-2)]);    % Interaction region
Matrix
L=diag([1 zeros(1,Np-1)]);R=diag([zeros(1,Np-1) 1]);zplus=i*1e-12; % Contact selection
Matrices

J=0.05;D=1e-20;ctr=1;sigB=zeros(4*Np);siginB=zeros(4*Np);
H0=2*t0*diag(ones(1,Np))-t0*diag(ones(1,Np-1),1)-t0*diag(ones(1,Np-1),-1); % Device
Hamiltonian
UB1=0*0.25;UB2=0*0.25;H0(N1,N1)=H0(N1,N1)+UB1;H0(N2,N2)=H0(N2,N2)+UB2;
    % Scattering potential

ii=1;dE=0.00125;
for EE=t0:-dE:t0
jj=1;
for HB=-0.5*t0:0.00625*t0:+0.5*t0
HS=J*(kron(sx,sx)+kron(sy,sy)+kron(sz,sz));            %Spin spin interaction
Hamiltonian
   H=kron(H0,eye(4))+kron(C,HS)+kron(eye(Np),kron([HB 0;0 -HB],eye(2)));  % Total
Hamiltonian including interaction and magnetic field
   ck=(1-(EE+zplus)/(2*t0));ka=acos(ck);
su=-t0*exp(i*ka)*0.5*(eye(2)+Pc*sz);                %Self Energy in z basis for upspin
sd=-t0*exp(i*ka)*0.5*(eye(2)-Pc*sz);                %Self Energy in z basis for downspin
s1uu=kron(U1*su*U1',[1 0;0 0]);s1ud=kron(U1*su*U1',[0 0;0 1]);  % Transformed Self
Energy
s1du=kron(U1*sd*U1',[1 0;0 0]);s1dd=kron(U1*sd*U1',[0 0;0 1]);  % Transformed Self
Energy
sig1uu=kron(L,s1uu);sig1ud=kron(L,s1ud);               % Total Self Energy applied
only at the contact points
sig1du=kron(L,s1du);sig1dd=kron(L,s1dd);               % Total Self Energy applied
only at the contact points
s2uu=kron(U2*su*U2',[1 0;0 0]);s2ud=kron(U2*su*U2',[0 0;0 1]);
s2du=kron(U2*sd*U2',[1 0;0 0]);s2dd=kron(U2*sd*U2',[0 0;0 1]);
sig2uu=kron(R,s2uu);sig2ud=kron(R,s2ud);
sig2du=kron(R,s2du);sig2dd=kron(R,s2dd);

gam1uu=i*(sig1uu-sig1uu');gam1ud=i*(sig1ud-sig1ud');       %Broadening
gam1du=i*(sig1du-sig1du');gam1dd=i*(sig1dd-sig1dd');       %Broadening
gam2uu=i*(sig2uu-sig2uu');gam2ud=i*(sig2ud-sig2ud');       %Broadening
```

```
gam2du=i*(sig2du-sig2du');gam2dd=i*(sig2dd-sig2dd');       %Broadening

%Self consistent calculation of Sigma_s
change=100;
while change>1e-6

G=inv((EE*eye(4*Np))-H-sig1uu-sig1ud-sig1du-sig1dd-sig2uu-sig2ud-sig2du-sig2dd-
sigB);
sigBnew=D*G;
change=ctr*(sum(sum(abs(sigBnew-sigB))))/(sum(sum(abs(sigBnew+sigB))));
sigB=sigB+ctr*(sigBnew-sigB);
end

% Self consistent calculation of Sigma_s^{in} to calculate Gn
   A=i*(G-G');change=100;jj   % Density of States
while change>1e-6
Gn=G*(gam1uu+siginB)*G';
siginBnew=D*Gn;
change=ctr*(sum(sum(abs(siginBnew-siginB))))/(sum(sum(abs(siginBnew+siginB))));
siginB=siginB+ctr*(siginBnew-siginB);
end

% Calculation of Transmission
TM1uu(jj)=real(trace(gam1uu*(A-Gn)));TM1ud(jj)=real(trace(gam1ud*Gn));
TM1du(jj)=real(trace(gam1du*Gn));TM1dd(jj)=real(trace(gam1dd*Gn));
TM2uu(jj)=real(trace(gam2uu*Gn));TM2ud(jj)=real(trace(gam2ud*Gn));
TM2du(jj)=real(trace(gam2du*Gn));TM2dd(jj)=real(trace(gam2dd*Gn));
B(jj)=HB;jj=jj+1;           % Magnetic Field
end
end

% Plots
hold on
h=plot(B,TM1dd+TM2dd+TM1du+TM2du,'b');
h=plot(B,TM2uu+TM1ud+TM2ud,'b');
```


B-field

References

These lectures are based on my books

Datta S., 1995, Electronic transport in mesoscopic systems, Cambridge University Press. ***Lectures 2.***

Datta S., 2005, Quantum Transport: Atom to Transistor, Cambridge University Press. ***Lectures 1,2.***

and recent tutorial articles

Datta S. 2005, "Spin Dephasing and Hot Spins", Proceedings of the International School of Physics "Enrico Fermi", Course CLX, From Nanostructures to Nanosensing Applications, Eds. A. D'Amico,G. Balestrino, and A. Paoletti, IOS, eprint: arXiv:condmat/0802.2067. ***Lectures 3.***

Datta S. 2008, "Nanodevices and Maxwell's demon", Lecture Notes in Nanoscale Science and Technology, Vol. 2, Nanoscale Phenomena: Basic Science to Device Applications, Eds. Z.K. Tang and P.Sheng, Springer, eprint: arXiv:condmat/0704.1623. ***Lectures 4.***

The ***simple model*** introduced in Lectures 1 is based on Chapter 1 of Datta (2005).

The ***NEGF-Landauer model*** introduced in Lectures 2 is based on

Datta S., 1989, Steady-state quantum kinetic equation. Phys. Rev., **B40**, 5830.

Datta S., 1990, A simple kinetic equation for steady-state quantum transport. Journal of Physics: Condensed Matter, **2**, 8023.

Meir Y. and Wingreen N.S. 1992. Landauer formula for the current through an interacting electron region. Phys. Rev. Lett. **68**, 2512.

Caroli C., Combescot R., Nozieres P. and Saint-James D. 1972. A direct calculation of the tunneling current: IV. Electron-phonon interaction effects. J.Phys.C: Solid State Phys. **5**, 21.

The ***Coulomb blockade model*** described in Lecture 5a is based on

Beenakker C.W.J., 1991, Theory of Coulomb blockade oscillations in the conductance of a quantum dot. Phys. Rev., **B44**, 1646.

For a different perspective on Coulomb blockade, see

Likharev K., 1999, Single electron devices and their applications. Proc. IEEE, **87**, 606.

A recent book on Spintronics that may be of interest.

Bandyopadhyay S. and Cahay M. 2008. Introduction to Spintronics, Taylor & Francis.