

*NCN-Intel Summer School on  
“Electronics from the Bottom-up”  
Purdue University, July 14-25, 2008*

**Nanoelectronics  
& the Meaning of Resistance  
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**July 14-18, 2008**

**Nanoelectronics**

**and the  
meaning of resistance**

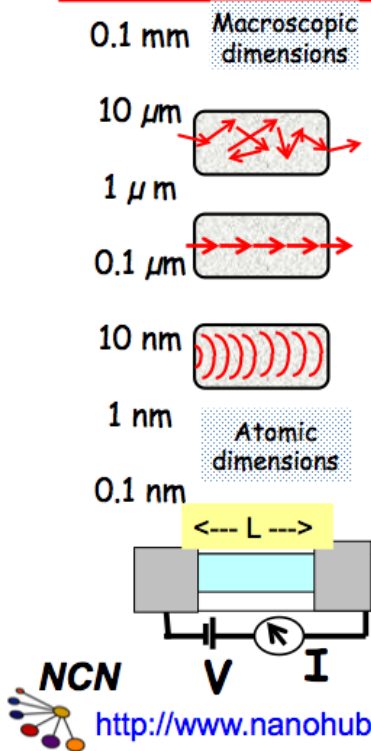
July 14: What and where is  
the resistance?

July 15: Quantum transport

July 16: Spins and magnets

July 17: Maxwell's demon

July 18: Correlations  
and entanglement

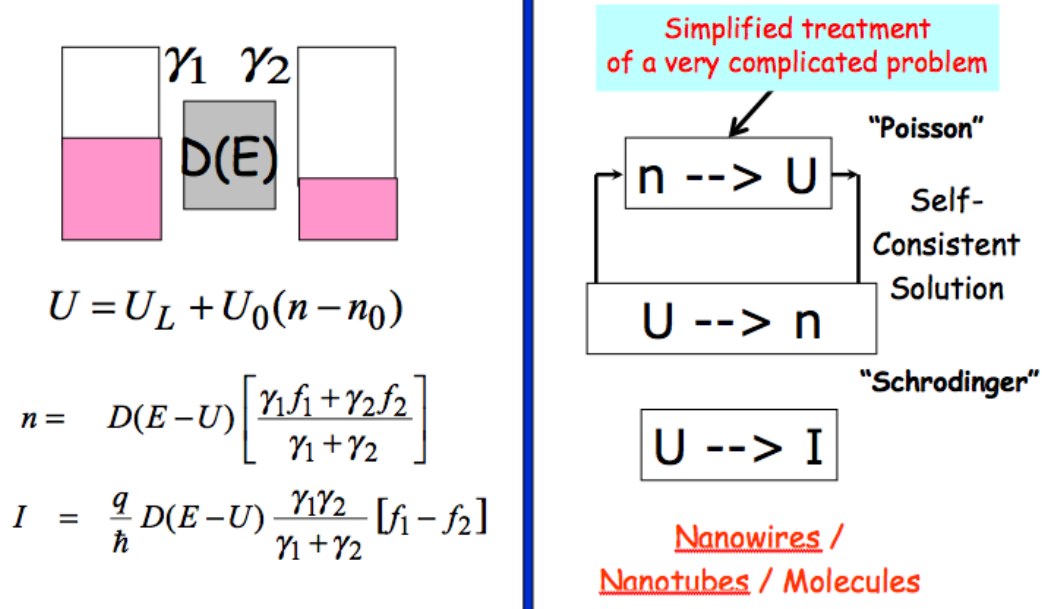


Supriyo Datta

PURDUE  
UNIVERSITY

## July 14: What and where is the resistance?

### Summary: Self-consistent field (scf) method



**Useful parameters:**  $q = 1.6 \times 10^{-19}$  coul,  $\hbar = 6.63 \times 10^{-34}$  joule-sec.

1. Calculate  $q^2/\hbar$ ,  $\hbar/q^2$ .
2. If  $\gamma = 1$  meV, calculate  $\gamma/\hbar$ ,  $q\gamma/\hbar$
3. If electron density  $n_s = 1 \times 10^{13}/\text{cm}^2$ , 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

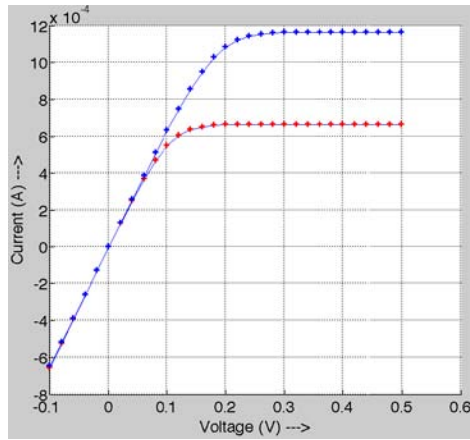
% Following calculates both currents and energy current at each bias point

% Bias
ii=1;dV=0.02;
for V=0:dV:0.5
UL=1e-12;
change=100;U=UL;
while change>1e-6 % Self-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
junction
volt(ii)=V;ii=ii+1;
end

```

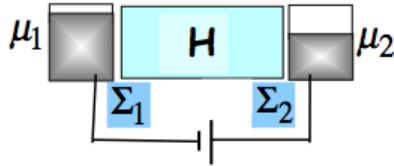
```
figure(1)  
hold on  
h=plot(volt,curr1,'b');h=plot(volt,curr2,'ro');
```



→  $U_0 = 0$

Day 2: Quantum transport

Coherent transport



- Semi-empirical
- First principles

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

$$\epsilon \rightarrow [H]$$

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

$$n \rightarrow [\rho]$$

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

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

Green function

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

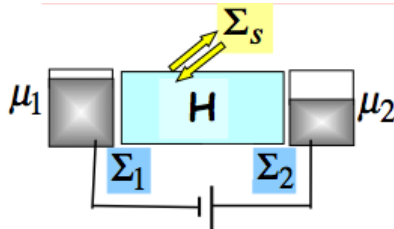
"Density of states"  $A = i[G - G^\dagger]$

"Electron density"

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

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

Incoherent transport



Green function

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

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

"Electron density"

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

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

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

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

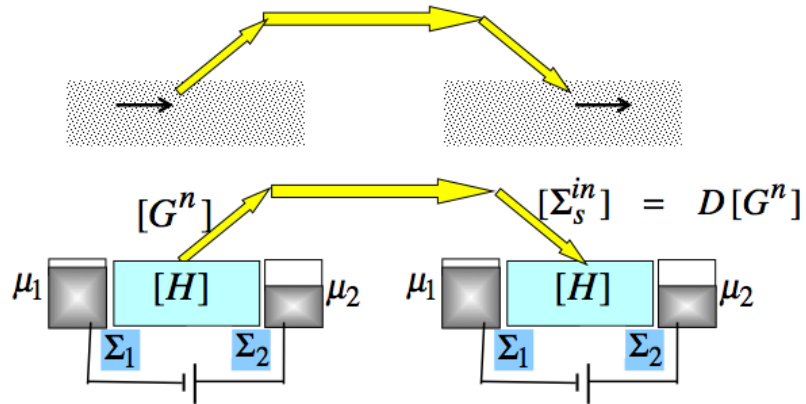
$$\epsilon \rightarrow [H]$$

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

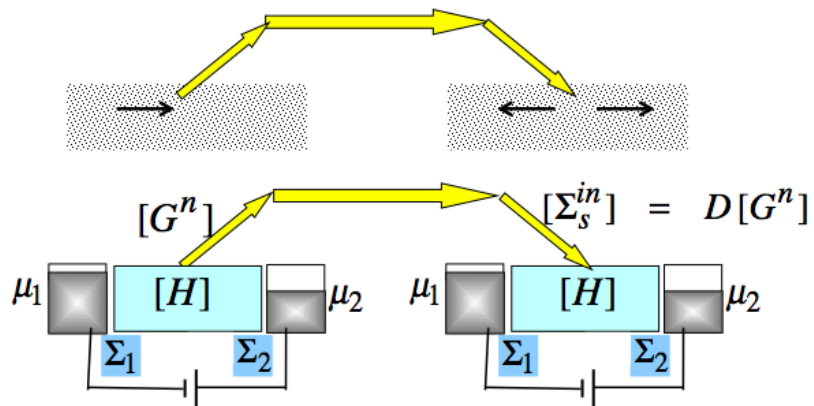
$$n \rightarrow [\rho]$$

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

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



Pure Phase Relaxation  $[\Sigma_s^{in}]_{ij} = d_p [G^n]_{ij}$



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)

$\hbar=1.06\text{e-}34$ ;  $q=1.6\text{e-}19$ ;  $m=0.2*9.1\text{e-}31$ ;  $a=1\text{e-}9$ ;  $t_0=(\hbar^2)/(2*m*(a^2)*q)$ ;

**%** Device structure

$N_p=25$ ;  $N_1=5$ ;  $N_2=21$ ;  $X=a*[0:1:N_p-1]$ ;

$L=\text{diag}([1 \text{ zeros}(1,N_p-1)])$ ;  $R=\text{diag}([ \text{zeros}(1,N_p-1) 1])$ ;

$D=1\text{e-}2$ ;  $\text{sigB}=\text{zeros}(N_p)$ ;  $\text{siginB}=\text{zeros}(N_p)$ ;

**%** Hamiltonian set-up

$H_0=2*t_0*\text{diag}(\text{ones}(1,N_p))-t_0*\text{diag}(\text{ones}(1,N_p-1),1)-t_0*\text{diag}(\text{ones}(1,N_p-1),-1)$ ;

$UB_1=1*0.25$ ;  $UB_2=1*0.25$ ;  $H_0(N_1,N_1)=H_0(N_1,N_1)+UB_1$ ;  $H_0(N_2,N_2)=H_0(N_2,N_2)+UB_2$ ;

$H=H_0$ ;

$ii=1$ ;  $dE=0.00125$ ;  $zplus=i*1\text{e-}12$ ;

for  $EE=0.001:dE:t_0$

**%**for  $EE=t_0:-dE:t_0$

$ck=(1-(EE+zplus)/(2*t_0))$ ;  $ka=\text{acos}(ck)$ ;  $s1=-t_0*\exp(i*ka)$ ;  $s2=-t_0*\exp(i*ka)$ ;

$\text{sig1}=\text{kron}(L,s1)$ ;  $\text{sig2}=\text{kron}(R,s2)$ ; **%** contact self energy

$\text{gam1}=i*(\text{sig1}-\text{sig1}')$ ;  $\text{gam2}=i*(\text{sig2}-\text{sig2}')$ ;

change=100;

**while** change>1e-6 **%** calculating G self-consistently

$G=\text{inv}((EE*\text{eye}(N_p))-H-\text{sig1}-\text{sig2}-\text{sigB})$ ;

$\text{sigBnew}=D*G$ ;

change=(sum(sum(abs(sigBnew-sigB)))/(sum(sum(abs(sigBnew+sigB))));

$\text{sigB}=\text{sigB}+0.25*(\text{sigBnew}-\text{sigB})$ ;

**end**

$A=\text{real}(\text{diag}(i*(G-G')))$ ; change=100; ii

**while** change>1e-6 **%** calculating Gn self-consistently

$G_n=G*(\text{gam1}+\text{siginB})*G'$ ;

$\text{siginBnew}=D*G_n$ ;

change=(sum(sum(abs(siginBnew-siginB)))/(sum(sum(abs(siginBnew+siginB))));

$\text{siginB}=\text{siginB}+0.25*(\text{siginBnew}-\text{siginB})$ ;

**end**

$T_{\text{coh}}(ii)=\text{real}(\text{trace}(\text{gam1}*G*\text{gam2}*G'))$ ;

$TM(ii)=\text{real}(\text{trace}(\text{gam2}*G_n))$ ;

$\mu(:,ii)=\text{real}(\text{diag}(G_n))./A$ ;  $E(ii)=EE$ ;  $ii=ii+1$ ;

**end**

**%**

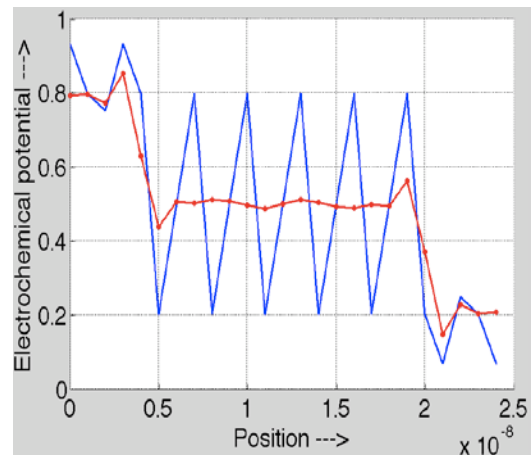
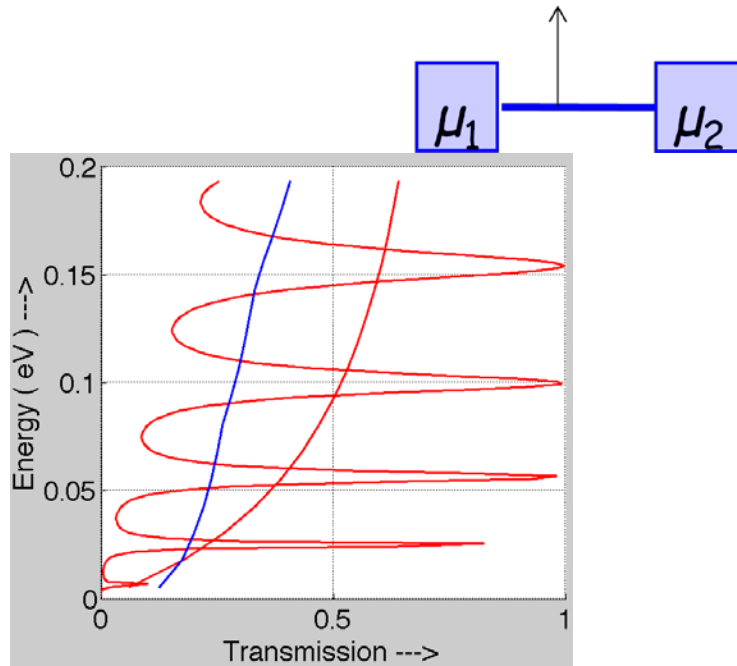
hold on

figure(1)

$h=\text{plot}(TM,E,'r')$ ;

figure(2)

$h=\text{plot}(X,\mu(:,1),'ro')$ ;





```

% 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
end

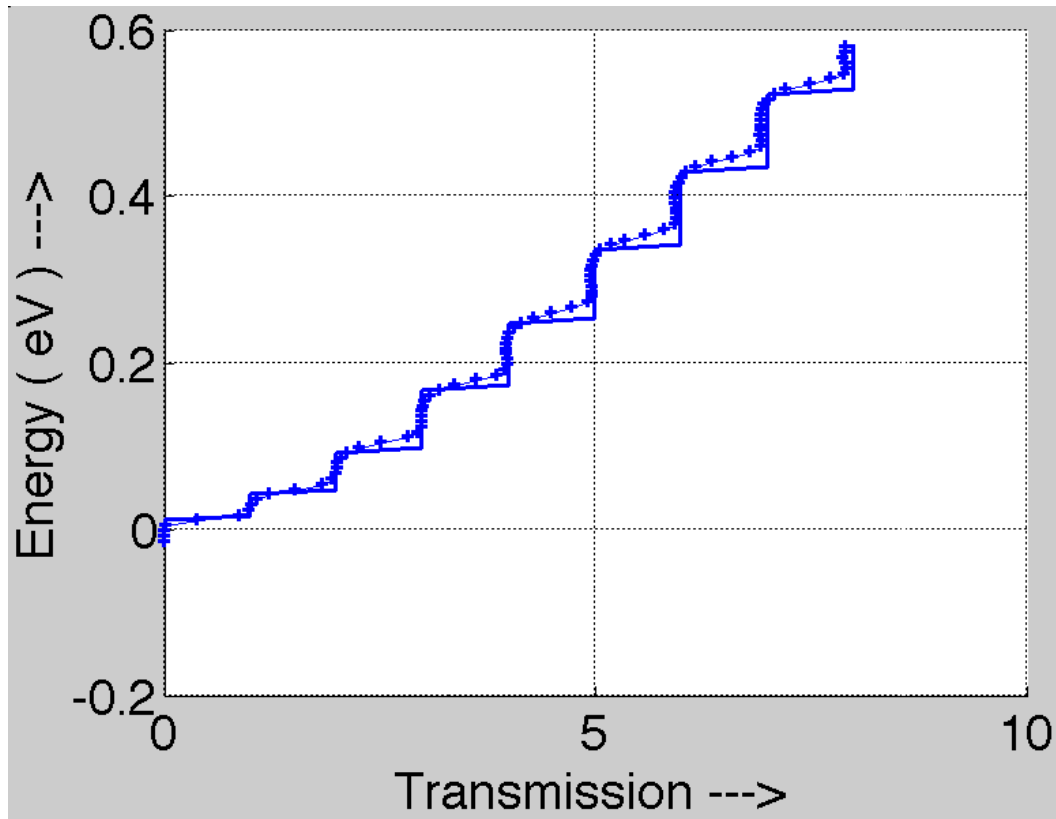
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```

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

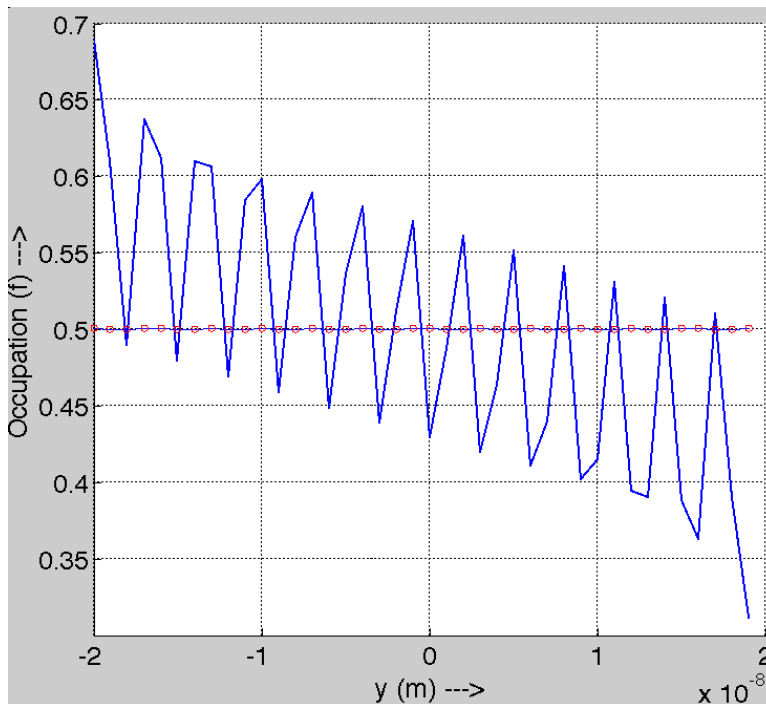
```

```

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+signinB)*G';
    signinBnew=D*Gn;
    change=ctr*(sum(sum(abs(signinBnew-signinB)))/(sum(sum(abs(signinBnew+signinB)))));
    signinB=signinB+0.25*ctr*(signinBnew-signinB);
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
signinB=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);
        siglu=kron(L,Utrans_L*su*Utrans_L');%Self Energy Matrix for Left Up-Spin
Contact
    end
end

```

---

```

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

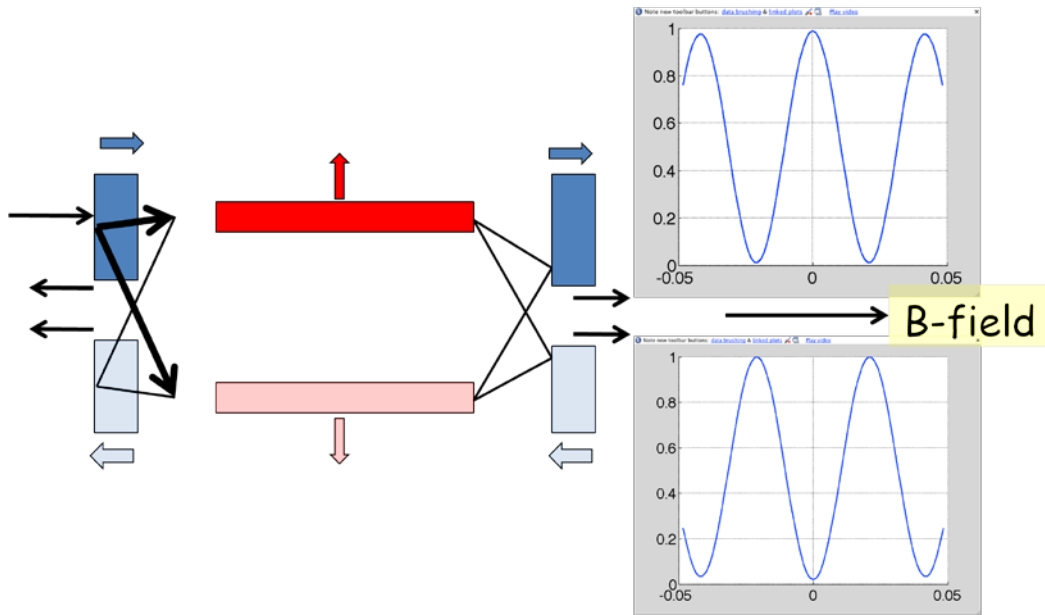
A=i*(G-G');%Evaluating Broadening function, A
change=100;jj

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

```



**% 3.2. Spin-NEGF code, 2D**

```

% Rashba term:  $s_x * k_y - s_y * k_x = (1/2/i/a) (e * i k_y a - e * -i k_y a) * s_x - (e * i k_x a - e * -i k_x a) * s_y$ 
% B-field:  $A_x = B y$ 
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);
signinB=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
end

```



```

end

change=1;
while change >5e-4
    Gs=inv(alpha-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(alpha-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

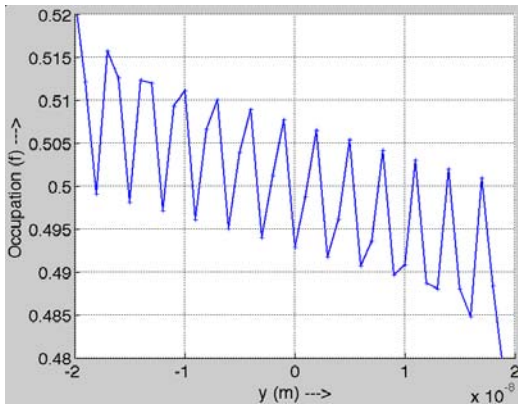
TM1(ii)=real(trace(gam1*(A-Gn)));
TM2(ii)=real(trace(gam2*Gn));
n(:,ii)=real(diag(Gn));%Electron Density
DD(:,ii)=real(diag(A));%Density of States
mu=n./DD;E(ii)=EE;ii
ii=ii+1;

end

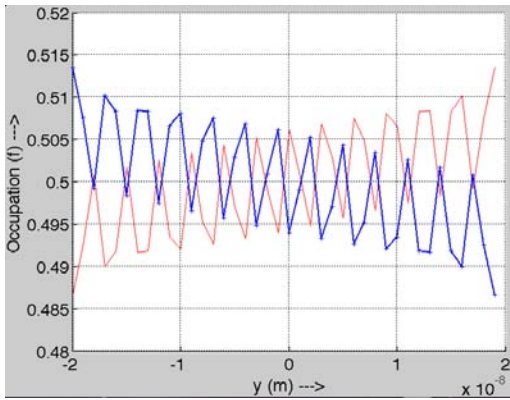
```

```
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
```

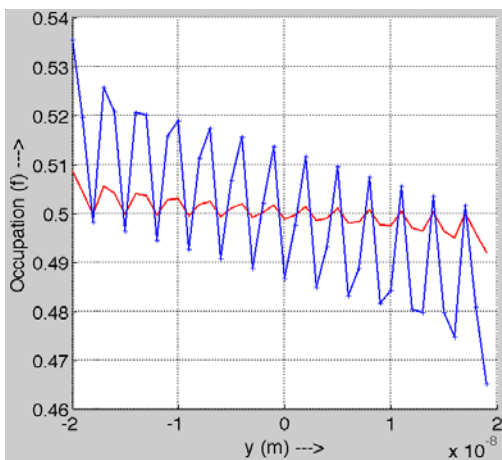
$$B = 1 T, \alpha = 0$$



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



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



## *Day 4: Maxwell's demon*

### **% 4.1. Seebeck and Peltier coefficients, simple code**

```

%%% Thermoelectric Effect %%%
% Finding Seebeck and Peltier coefficient
% 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 function at hot(left)
f2=1./(1+exp((E-mu2)./kT2)); % Fermi function 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];

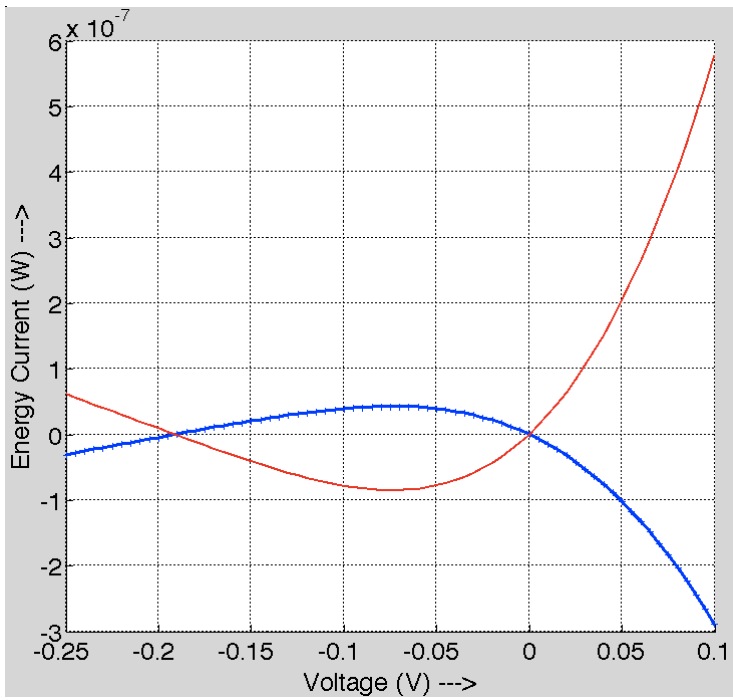
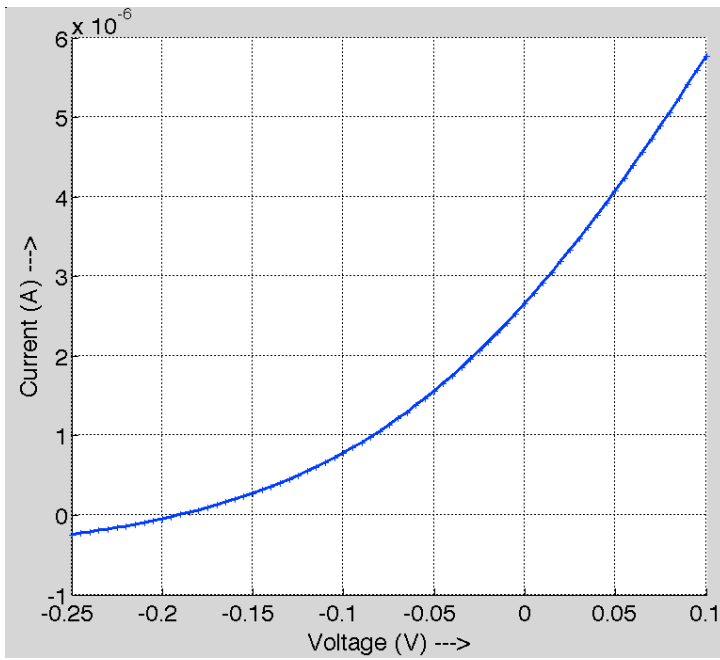
ii=1;for V=-0.2:dE:0.1
% for V=0.05:0.2*kT:0.05
mu1=(0.5)*V;mu2=(-0.5)*V;
f1d=1./(1+exp((E-mu1)./kT));f1u=f1d;
f2d=1./(1+exp((E-mu2)./kT));f2u=f2d;
fu=f1u;fd=f2d;% Initial guess

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

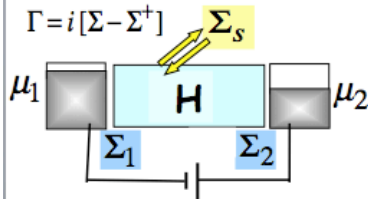
%Sum over energy
I1(ii)=(dE*sum((g1u*(f1u-fu)+(g1d*(f1d-fd))));
I2(ii)=dE*sum((g2u*(fu-f2u)+(g2d*(fd-f2d))));
IE1(ii)=dE*sum((E-mu1).*((g1u*(f1u-fu)+(g1d*(f1d-fd))));
IE2(ii)=dE*sum((mu2-E).*((g2u*(fu-f2u)+(g2d*(fd-f2d))));
Idu(ii)=dE*g*sum(fd.*(1-fu));Iud(ii)=dE*g*sum(fu.*(1-fd));
volt(ii)=V;ii=ii+1;

end

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



## 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"

$$\begin{aligned} A &= G^n + G^p \\ &= i[G - G^+] \end{aligned}$$

Broadening

$$\begin{aligned} [\Gamma_s] &= [\Sigma_s^{in} + \Sigma_s^{out}] \\ &= i[\Sigma_s - \Sigma_s^+] \end{aligned}$$

Dephasing

$$\begin{aligned} [\Sigma_s^{in}(E)] &= [[D(\varepsilon)]][G^n(E - \varepsilon)] \\ [\Sigma_s^{out}(E)] &= [[D(-\varepsilon)]]^T [G^p(E - \varepsilon)] \\ [\Sigma_s(E)] &= [h(E)] - \frac{i}{2}[\Gamma_s(E)] \end{aligned}$$


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## 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);signinB=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

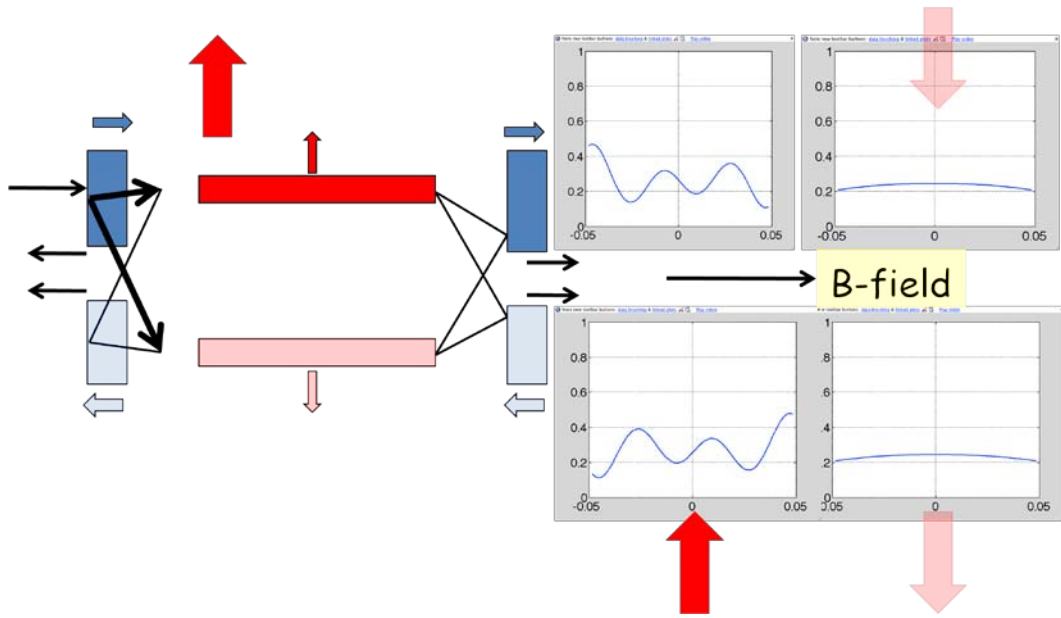
G=inv((EE*eye(4*Np))-H-sig1uu-sig1ud-sig1du-sig1dd-sig2uu-sig2ud-sig2du-sig2dd-
sigB);
sigBnew=D*G;
change=ctr*(sum(sum(abs(sigBnew-sigB)))/(sum(sum(abs(sigBnew+sigB)))));
sigB=sigB+ctr*(sigBnew-sigB);
end

% 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+signinB)*G';
signinBnew=D*Gn;
change=ctr*(sum(sum(abs(signinBnew-signinB)))/(sum(sum(abs(signinBnew+signinB)))));
signinB=signinB+ctr*(signinBnew-signinB);
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');

```



## References

*These lectures are based on my books*

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

*and recent tutorial articles*

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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

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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.