

## ECE 659, TAKE-HOME EXAM **SOLUTION**

All ten questions carry 20 points each,  $10 \times 20 = 200$

The MATLAB-based problems in this exam have been chosen to illustrate and solidify the concepts covered in the different exams as indicated below.

*Based on Exam 2 (Feb.4) concepts:*

*Target date*

*TH1: Hydrogen atom, 1s energy level*

*Feb.22*

*TH2: Helium atom, 1s energy level*

*Feb.25*

*TH3: Principle of bandstructure*

*Feb.27*

*Based on Exam 3 (Feb.20) concepts:*

*TH4: Resonant tunneling*

*Mar.1*

*TH5: Potential drop across a scatterer*

*Mar.4*

*Based on Exam 4 (Mar.8) concepts:*

*TH6: Quantized conductance: Modes or subbands*

*Mar.19*

*TH7: Quantized conductance in graphene, CNT*

*Mar.22*

*TH8: Quantum Hall effect and edge states*

*Mar.29*

*Based on Exam 5 (Apr. 5) concepts:*

*TH9: Non-local spin voltage*

*Apr.12*

*TH10: Voltage controlled spin precession ("Spin Transistor")*

*Apr.19*

**References:** For TH1-TH3 you may want to look at Chapters 2, 3 and 5 of QTAT: "Quantum Transport: Atom to Transistor" Cambridge, 2005. If you do not have access to a copy please let me know. Other problems are largely based on LNE: "Lessons from Nanoelectronics" World Scientific, 2012 (manuscript version can be downloaded from Blackboard).

I have included a copy of my own MATLAB code for each problem (except for TH3 for which the code is straightforward) that you can use for guidance in writing your own codes. But please make sure that you understand any code that you submit, in the sense that you can explain how they are supposed to work if called on to do so.

### TH1: Hydrogen atom

The energy levels of a hydrogen atom can be obtained by solving the Schrodinger equation *analytically*, no computer is needed. As such it is a nice benchmark problem that we can use to check our numerical code. However, a few analytical steps are needed to get from the full 3-D Schrodinger equation to the 1D radial Schrodinger equation which we solve numerically on a computer.

**Step 1:** Start from 3D Schrodinger equation for a hydrogen atom in spherical coordinates

$$E \psi(\vec{r}) = \left( -\frac{\hbar^2}{2m} \nabla^2 - \frac{q^2}{4\pi\epsilon_0 r} \right) \psi(\vec{r}) \quad (1.1)$$

$$\nabla^2 \equiv \left( \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \left( \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right) \quad (1.2)$$

(a) Show that a solution of the form  $\psi(\vec{r}) = R(r) Y_\ell^m(\theta, \phi)$  satisfies (1.1) provided

$$E R(r) = \left( -\frac{\hbar^2}{2m} \left( \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) - \frac{q^2}{4\pi\epsilon_0 r} + \frac{\hbar^2 l(l+1)}{2m r^2} \right) R(r) \quad (1.3)$$

$Y_\ell^m(\theta, \phi)$  are known as the spherical harmonics. There should be a Wikipedia page where the actual functions for different values of  $(\ell, m)$  are listed, but to obtain (1.3) from (1.1) you only need to make use of the fact that all  $Y_\ell^m(\theta, \phi)$  satisfy the following differential equation:

$$\left( \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right) Y_\ell^m = -\ell(\ell+1) Y_\ell^m \quad (1.4)$$

**SOLUTION:** Substituting

$$\psi(\vec{r}) = R(r) Y_\ell^m(\theta, \phi)$$

into (1.1) and making use of (1.4) we have

$$E R(r) Y_\ell^m(\theta, \phi) = \left( -\frac{\hbar^2}{2m} \left( \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) - \frac{q^2}{4\pi\epsilon_0 r} + \frac{\hbar^2 l(l+1)}{2m r^2} \right) R(r) Y_\ell^m(\theta, \phi)$$

We can cancel  $Y_\ell^m(\theta, \phi)$  term from both sides to get (1.3):

**Step 2:**

(b) Show that a solution of the form  $R(r) = \frac{f(r)}{r}$  satisfies (1.3) provided

$$E f(r) = \left( -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} - \frac{q^2}{4\pi\epsilon_0 r} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} \right) f(r) \quad (1.5)$$

which is the equation we will solve numerically to obtain the energy levels.

**SOLUTION:**

We know that

$$\begin{aligned} \left( \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) \frac{f(r)}{r} &= \left( \frac{d}{dr} + \frac{2}{r} \right) \frac{d}{dr} \frac{f(r)}{r} = \left( \frac{d}{dr} + \frac{2}{r} \right) \left( \frac{f'}{r} - \frac{f}{r^2} \right) \\ &= \frac{f''}{r} - \frac{f'}{r^2} - \frac{f'}{r^2} + \frac{2f}{r^3} + \frac{2f'}{r^2} - \frac{2f}{r^3} = \frac{f''}{r} \end{aligned}$$

Now substituting  $R(r) = f(r)/r$  in (1.3), we have (1.5).

**Step 3:** We could solve (1.5) with  $\ell=0$  for the “s” levels, with  $\ell=1$  for the “p” levels with  $\ell=2$  for the “d” levels etc. But we will focus only on the first one ( $\ell=0$ ).

(c) Show that a solution of the form  $f(r) = r e^{-r/a_0}$  satisfies (1.5) provided

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m q^2} \text{ and that the corresponding energy } E \text{ is equal to } \frac{q^2}{8\pi\epsilon_0 a_0}$$

**SOLUTION:**

For 1s level  $l = 0$ . Substituting  $f(r) = r e^{-r/a_0}$  into (1.5)

$$\begin{aligned} E r e^{-r/a_0} &= \left( -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} - \frac{q^2}{4\pi\epsilon_0 r} \right) r e^{-r/a_0} \\ &= \left( -\frac{\hbar^2}{2ma_0} \frac{d^2}{d\rho^2} - \frac{q^2}{4\pi\epsilon_0 \rho} \right) \rho e^{-\rho} \quad , \quad \rho \equiv r / a_0 \end{aligned}$$

$$= \left( -\frac{\hbar^2}{2ma_0} \frac{d}{d\rho} \right) (1-\rho)e^{-\rho} - \frac{q^2}{4\pi\epsilon_0} e^{-\rho}$$

$$= \frac{\hbar^2}{2ma_0} (2-\rho)e^{-\rho} - \frac{q^2}{4\pi\epsilon_0} e^{-\rho}$$

$$E a_0 \rho e^{-\rho} = \left( -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} - \frac{q^2}{4\pi\epsilon_0 r} \right) r e^{-r/a_0} = -\frac{\hbar^2}{2ma_0} \rho e^{-\rho} + \underbrace{\left( \frac{\hbar^2}{ma_0} - \frac{q^2}{4\pi\epsilon_0} \right)}_{=0} e^{-\rho}$$

$$\frac{\hbar^2}{ma_0} = \frac{q^2}{4\pi\epsilon_0} \rightarrow a_0 = \frac{4\pi\epsilon_0 \hbar^2}{mq^2}$$

$$E = -\frac{\hbar^2}{2ma_0^2} = -\frac{q^2}{8\pi\epsilon_0 a_0}$$

**Step 4: (d)** Here is the MATLAB code I wrote to solve (1.5) for the eigenvalues.

```
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=(2e-10/Np);% Np is number of points, a is range
R=a*[1:1:Np];t0=(hbar^2)/(2*m*(a^2))/q;

%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;U=diag(U);

[V,D]=eig(K+U);D=diag(D);E=D(1); % Lowest eigenvalue
psi=V(:,1);P=psi.*conj(psi);% Corresponding wavefunction
P1s=(4*a/(a0^3))*R.*R.*exp(-2*R./a0);%Analytical solution

[E -E0], % Numerical and analytical eigenvalue

hold on
h=plot(R,P,'k');
h=plot(R,P1s,'ko');
```

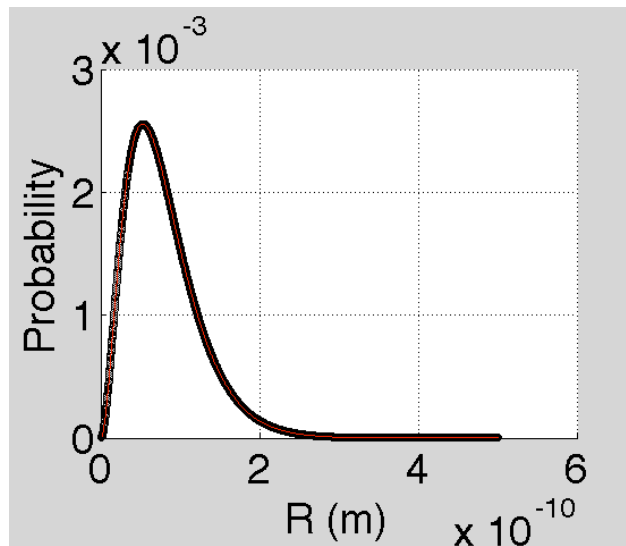
grid on

This code gives a lowest energy eigenvalue of -12.98 eV as compared to the analytical result of -13.59 eV. Please write a code with an increased number of points ( $N_p$ ) and increased radial range ( $N_p \cdot a$ ) that gives a more accurate numerical result  $\sim -13.59$  eV.

### **SOLUTION:**

For better convergence we have changed  $N_p=2000$  and  $a=5e-10/N_p$ .

This gives  $E = -13.5915$  eV and good agreement of wavefunction squared (probability) with analytical result.



### TH2: Helium atom

Calculating the energy levels for anything with more than one electron requires us to include a potential  $U_{\text{scf}}(r)$  due to the other electron(s) in addition to the potential  $U_N(r)$  due to the positive nucleus. The potential due to the other electron(s) needs to be calculated *self-consistently* since the charge distribution itself depends on the wavefunctions obtained from the solution of the Schrodinger equation. Here is the code I wrote to calculate the lowest energy level for a Helium atom which has two electrons.

```
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=500;a=(5e-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

% Self-consistent calculation
Uscf=zeros(1,Np);change=1;
while change>1e-3
[V,D]=eig(T+diag(UN+Uscf));D=diag(D);
psi=V(:,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
E=D(1), UscfAverage=sum(Uscf.*P)

h=plot(R,Uscf,'k');
xlabel(' R (m) --> ')
ylabel(' Uscf (eV) --> ')
grid on
```

- (a) Please write a code and use it to calculate the energy of the lowest level for a Helium atom (b)  $E_0'$ , ignoring  $U_{\text{scf}}$ , and (c)  $E_0$ , including  $U_{\text{scf}}$ . ?

**SOLUTION:**

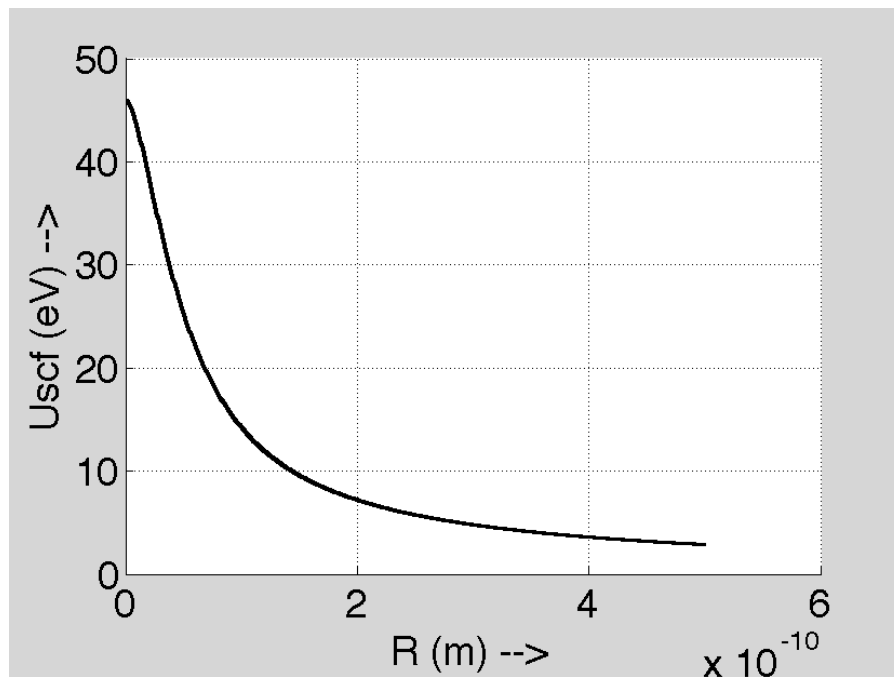
For Part (b), set  $U_{\text{new}}$  equal to zero.

(d) The difference  $E_0 - E_0'$  represents the increase in the potential of the atom due to a single electron. Compare this single electron charging energy with the average value of  $U_{\text{scf}}$

$$E_0' \text{ (ignoring } U_{\text{scf}} \text{)} = -54.35 \text{ eV}$$

$$E_0 \text{ (including } U_{\text{scf}} \text{)} = -24.94 \text{ eV}$$

$E_0 - E_0' = 29.41 \text{ eV}$ , a little larger than the spatially averaged  $\langle U_{\text{scf}} \rangle$ , which equals 27.88 eV.



### TH3: Principle of bandstructure

We have seen in class how  $E(k)$  relations can be used to write down the eigenvalues of a periodic matrix analytically. We would like to test it with a few simple examples.

(a) Write a MATLAB code to find the eigenvalues of the periodic matrix

$$\begin{bmatrix} \varepsilon & t & 0 & 0 & 0 & t \\ t & \varepsilon & t & 0 & 0 & 0 \\ 0 & t & \varepsilon & t & 0 & 0 \\ 0 & 0 & t & \varepsilon & t & 0 \\ 0 & 0 & 0 & t & \varepsilon & t \\ t & 0 & 0 & 0 & t & \varepsilon \end{bmatrix}$$

with  $\varepsilon = 0, t = -1$  and compare with those predicted from the  $E(k)$  relation:

$$\varepsilon + 2t \cos[-3 \quad -2 \quad -1 \quad 0 \quad +1 \quad +2].*2\pi/6 \quad (3.1)$$

(b) Use MATLAB to find the eigenvalues of the matrix with *box boundary conditions*

$$\begin{bmatrix} \varepsilon & t & 0 & 0 & 0 & 0 \\ t & \varepsilon & t & 0 & 0 & 0 \\ 0 & t & \varepsilon & t & 0 & 0 \\ 0 & 0 & t & \varepsilon & t & 0 \\ 0 & 0 & 0 & t & \varepsilon & t \\ 0 & 0 & 0 & 0 & t & \varepsilon \end{bmatrix}$$

Write down the appropriate equation to replace (3.1) that will describe these eigenvalues and compare.

(c) Use MATLAB to find the eigenvalues of the periodic matrix

$$\begin{bmatrix} \varepsilon & t_1 & 0 & 0 & 0 & t_2 \\ t_1 & \varepsilon & t_2 & 0 & 0 & 0 \\ 0 & t_2 & \varepsilon & t_1 & 0 & 0 \\ 0 & 0 & t_1 & \varepsilon & t_2 & 0 \\ 0 & 0 & 0 & t_2 & \varepsilon & t_1 \\ t_2 & 0 & 0 & 0 & t_1 & \varepsilon \end{bmatrix}$$

with  $\varepsilon = 0, t_1 = -1.5, t_2 = -0.5$  and compare with those predicted from the relation:

$$\begin{aligned} \varepsilon + \sqrt{t_1^2 + t_2^2 + 2t_1t_2 \cos[-1 \quad 0 \quad +1].*2\pi/3} \\ \varepsilon - \sqrt{t_1^2 + t_2^2 + 2t_1t_2 \cos[-1 \quad 0 \quad +1].*2\pi/3} \end{aligned} \quad (3.2)$$

Explain how you would obtain Eq.(3.2) by deriving an  $E(k)$  relation using the principles of bandstructure.



**SOLUTION:**

```
clear all
ep=0;t=-1;
```

```
% (a) Periodic boundary condition
```

```
HP=[ep t 0 0 0 t;
    t ep t 0 0 0;
    0 t ep t 0 0;
    0 0 t ep t 0;
    0 0 0 t ep t;
    t 0 0 0 t ep];
```

```
[V,D]=eig(HP);D=transpose(diag(D)), % Numerical
```

```
ka=2*pi*[-3 -2 -1 0 1 2]/6; ep+2*t*cos(ka), % Analytical
```

```
% (b) Box boundary condition
```

```
HB=[ep t 0 0 0 0;
    t ep t 0 0 0;
    0 t ep t 0 0;
    0 0 t ep t 0;
    0 0 0 t ep t;
    0 0 0 0 t ep];
```

```
[V,D]=eig(HB);D=transpose(diag(D)), % Numerical
```

```
ka=pi*[1 2 3 4 5 6]/7;ep+2*t*cos(ka), % Analytical
```

```
% (c) Unit cell with two sites, PBC
```

```
t1=-1.5;t2=-0.5;% t1=-0.5;t2=-1.5;
```

```
HB=[ep t1 0 0 0 t2;
    t1 ep t2 0 0 0;
    0 t2 ep t1 0 0;
    0 0 t1 ep t2 0;
    0 0 0 t2 ep t1;
    t2 0 0 0 t1 ep];
```

```
[V,D]=eig(HB);D=transpose(diag(D)), % Numerical
```

```
ka=2*pi*[-1 0 1]/3;
```

```
[ep-sqrt(t1^2+t2^2+2*t1*t2*cos(ka)) ep+sqrt(t1^2+t2^2+2*t1*t2*cos(ka))],
% Analytical
```

*Eigenvalues from MATLAB and from analytical expression match well.*

$$(a) \quad \varepsilon + 2t \cos[-3 \quad -2 \quad -1 \quad 0 \quad +1 \quad +2].*2\pi/6$$

$$\begin{matrix} -2.0000 & -1.0000 & -1.0000 & 1.0000 & 1.0000 & 2.0000 \end{matrix}$$

$$(b) \quad \varepsilon + 2t \cos[1 \quad 2 \quad 3 \quad 4 \quad 5 \quad 6].*\pi/7$$

$$\begin{matrix} -1.8019 & -1.2470 & -0.4450 & 0.4450 & 1.2470 & 1.8019 \end{matrix}$$

$$(c) \quad \varepsilon \pm \sqrt{t_1^2 + t_2^2 + 2t_1 t_2 \cos[-1 \quad 0 \quad +1].*2\pi/3}$$

$$\begin{matrix} -2.0000 & -1.3229 & -1.3229 & 1.3229 & 1.3229 & 2.0000 \end{matrix}$$

*Derivation of analytical expression in (c) :*

$$h(k) = \begin{bmatrix} 0 & t_2 \\ 0 & 0 \end{bmatrix} e^{-ikb} + \begin{bmatrix} \varepsilon & t_1 \\ t_1 & \varepsilon \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ t_2 & 0 \end{bmatrix} e^{+ikb} = \begin{bmatrix} \varepsilon & t_1 + t_2 e^{-ikb} \\ t_1 + t_2 e^{+ikb} & \varepsilon \end{bmatrix}$$

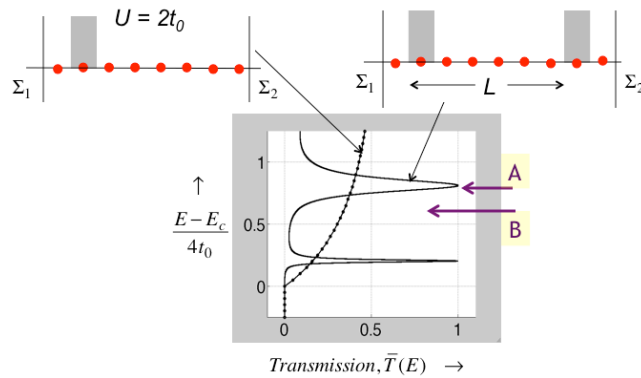
$$E(k) = \varepsilon \pm \sqrt{(t_1 + t_2 e^{+ikb})(t_1 + t_2 e^{-ikb})}$$

$$= \varepsilon \pm \sqrt{t_1^2 + t_2^2 + 2t_1 t_2 \cos kb}$$

#### TH4: Resonant tunneling

Fig.20.4 in LNE shows that resonant tunneling structures with two barriers exhibit resonant peaks in the transmission. Fig.20.4 →

Here is my code with two barriers of height  $2*t_0$  located at sites 3 and 9:



```
clear all
t0=1;Np=11;X=[0:1:Np-1];
L=diag([1 zeros(1,Np-1)]);R=diag([zeros(1,Np-1) 1]);
zplus=i*1e-12;

H0=2*t0*diag(ones(1,Np))-t0*diag(ones(1,Np-1),1)...
-t0*diag(ones(1,Np-1),-1);
N1=3;N2=9;UB1=2*t0;UB2=2*t0;
H0(N1,N1)=H0(N1,N1)+UB1;H0(N2,N2)=H0(N2,N2)+UB2;H=H0;

VV=0;UV=linspace(0,-VV,Np); % Linear potential

ii=1;dE=5e-4; for EE=[-0.25:dE:1.25]*t0
    ck=(1-(EE-UV(1)+zplus)/(2*t0));ka=acos(ck);
    s1=-t0*exp(i*ka);sig1=kron(L,s1);
    ck=(1-(EE-UV(Np)+zplus)/(2*t0));ka=acos(ck);
    s2=-t0*exp(i*ka);sig2=kron(R,s2);
    gam1=i*(sig1-sig1');gam2=i*(sig2-sig2');

    G=inv((EE*eye(Np))-H-diag(UV)-sig1-sig2);
    Tcoh(ii)=real(trace(gam1*G*gam2*G'));
    E(ii)=EE/t0;ii=ii+1;
end

h=plot(Tcoh,E,'k');
set(h,'linewidth',[3.0])
set(gca,'FontSize',[36])
axis([-0.1 1.1 -0.25 1.25]);
grid on
```

- (a) Write a code to calculate the transmission for two barriers of height  $2t_0$  located at sites 3 and 11. Compare the location of each of the two peaks with the energy levels for a box of length  $L = (11-3)*a$  and for a box of length  $(11-3+1)*a$ .

Repeat with two barriers of height  $t_0/2$  located at sites 3 and 9.

**SOLUTION:**

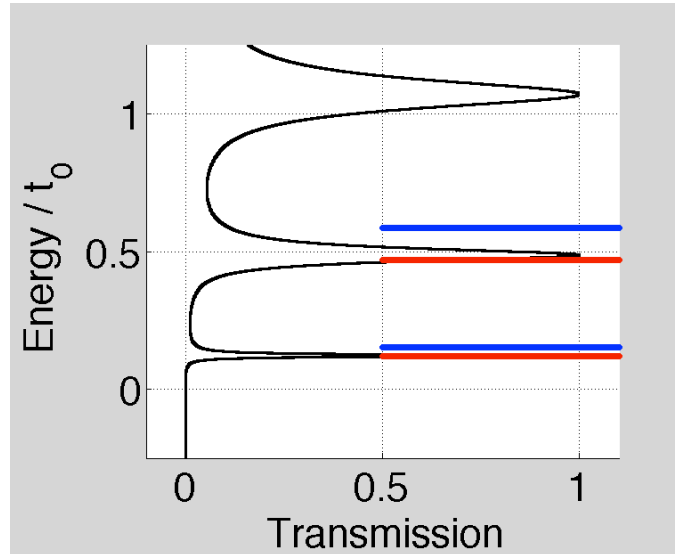
```

E1 = 2*t0*(1-cos(pi/(N2-N1+1))); % Plotted in Red
E2 = 2*t0*(1-cos(2*pi/(N2-N1+1))); % Plotted in Red
E1a = 2*t0*(1-cos(pi/(N2-N1))); % Plotted in Blue
E2a = 2*t0*(1-cos(2*pi/(N2-N1))); % Plotted in Blue

```

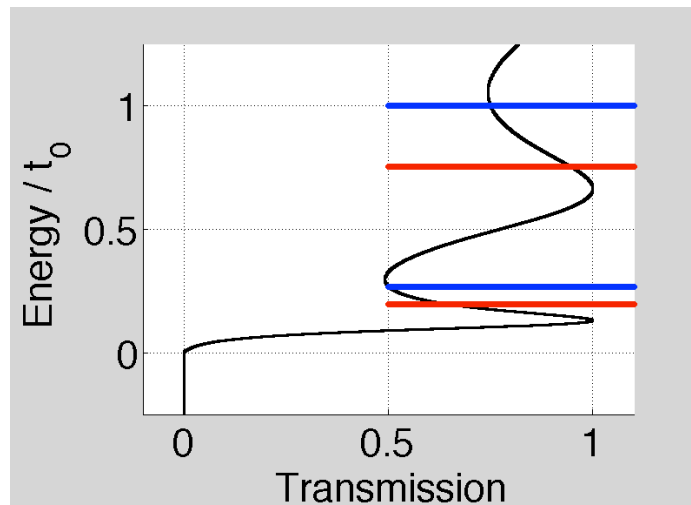
*(a) Change N2 to 11.*

*Both peaks match red (the larger “box”) better.*



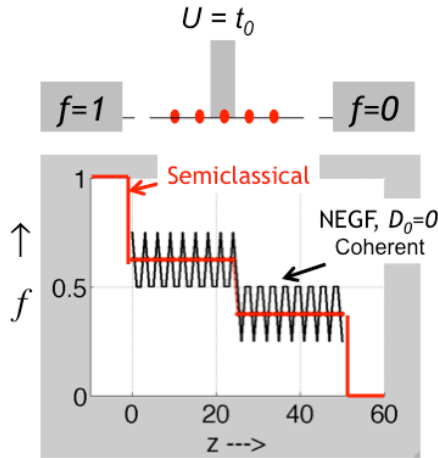
*(b) Change N2 back to 9, and UB1 and UB2 to  $t_0 / 2$ .*

*Peaks lower than the red because the smaller barriers mean that the wavefunction spreads out more making the “box” effectively wider.*

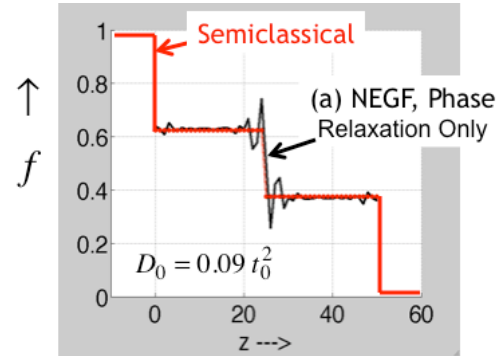


### TH5: Potential drop across a scatterer

Fig.20.6 in LNE shows the electrochemical potential profile calculated from a coherent model while Fig.20.7a shows the profile calculated including phase relaxation.



**Fig.20.6**



**Fig.20.7a**

Below is my code for the purpose:

```
t0=1;Np=51;X=[0:1:Np-1];Nh=floor(Np/2);
L=diag([1 zeros(1,Np-1)]);R=diag([zeros(1,Np-1) 1]);
zplus=i*1e-12;D=9e-2*t0^2;

sigB=zeros(Np);siginB=zeros(Np);

H0=2*t0*diag(ones(1,Np))-t0*diag(ones(1,Np-1),1)...
-t0*diag(ones(1,Np-1),-1);
N1=Nh+1;UB1=1*t0;
H0(N1,N1)=H0(N1,N1)+UB1;H=H0;

EE=t0;
ck=(1-(EE+zplus)/(2*t0));ka=acos(ck);
v=2*t0*sin(ka);
% Semiclassical profile
T=real(v^2/(UB1^2+v^2));R1=(1-T)/T;
TT=real(v^2/(D+v^2));R2=1*(1-TT)/TT;
RR=[0.5 R2*ones(1,Nh) R1 R2*ones(1,Nh) 0.5];
RR=cumsum(RR);Vx=ones(1,Np+2)-(RR./RR(Np+2));
Fclass=Vx([2:Np+1]);
```

```

%Based on resistance estimates

s1=-t0*exp(i*ka);sig1=kron(L,s1);
ck=(1-(EE+zplus)/(2*t0));ka=acos(ck);
s2=-t0*exp(i*ka);sig2=kron(R,s2);
gam1=i*(sig1-sig1');gam2=i*(sig2-sig2');

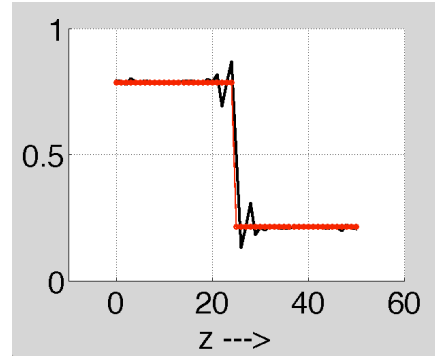
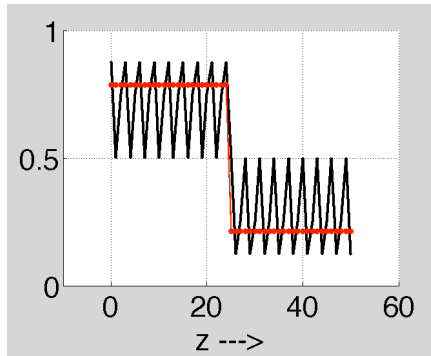
G=inv((EE*eye(Np))-H-sig1-sig2);
Tcoh=real(trace(gam1*G*gam2*G'));

change=100;% Including dephasing in the calculation
while change>1e-6
    G=inv((EE*eye(Np))-H-sig1-sig2-sigB);
    sigBnew=diag(diag(D*G));%sigBnew=D*G;
    change=sum(sum(abs(sigBnew-sigB)));
    sigB=sigB+0.25*(sigBnew-sigB);
end
A=real(diag(i*(G-G')));change=100;
while change>1e-6
    Gn=G*(gam1+signinB)*G';
    signinBnew=diag(diag(D*Gn));%signinBnew=D*Gn;
    change=sum(sum(abs(signinBnew-signinB)));
    signinB=signinB+0.25*(signinBnew-signinB);
end
F=real(diag(Gn))./A;

hold on
h=plot(X,F,'k');
set(h,'linewidth',[3.0])
h=plot(X,Fclass,'r-o');
set(h,'linewidth',[1.2])
set(gca,'FontSize',[36])
xlabel(' z ----> ')
grid on
axis([-10 60 0 1])

```

- (a) Write a code for the same structure but with a barrier of height  $2*t_0$  (instead of  $t_0$ ) and obtain plots like Figs. 20.6 and 20.7a.
- (b) Explain how you would estimate semiclassically the fraction of the total potential that is dropped across the barrier.

**SOLUTION:**

(b)  $E = 2t_0(1 - \cos ka) = t_0 \rightarrow ka = \pi / 3$

$$T = \frac{(\hbar v / a)^2}{U_B^2 + (\hbar v / a)^2} = \frac{(2t_0 \sin ka)^2}{U_B^2 + (2t_0 \sin ka)^2} = \frac{3}{7}$$

$$\frac{1-T}{T} = \frac{4}{3} \rightarrow \text{Normalized resistance of scatterer}$$

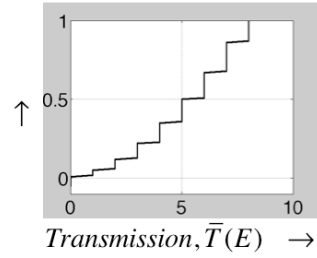
Steps proportional to  $1/2 : 4/3 : 1/2 = 3 : 8 : 3$   
 $= 0.215 : 0.57 : 0.215$

### TH6: Modes or subbands

Fig.21.1c in LNE shows the transmission versus energy for a 2D ballistic conductor with 25 lattice sites along the width.

(c) Numerical Result

$$\frac{E - E_c}{t_0}$$



Below is my code:

Fig.21.1c →

```
clear all
%Constants (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;qh=q/hbar;B=0;

%inputs
a=2.5e-9;t0=1;
NW=25;Np=1;L=zeros(Np);R=L;L(1,1)=1;R(Np,Np)=1;zplus=i*1e-12;

%Hamiltonian
al=4*t0;by=-t0;bx=-t0;
alpha=kron(eye(NW),al)+kron(diag(ones(1,NW-1),+1),by)+kron(diag(ones(1,NW-1),-1),by');
alpha=alpha+diag([1:1:NW].*0);
alpha=alpha+diag([zeros(1,8) 0*ones(1,9) zeros(1,8)]);
beta=kron(diag(exp(i*qh*B*a*a*[1:1:NW])),bx);
H=kron(eye(Np),alpha);
if Np>1
H=H+kron(diag(ones(1,Np-1),+1),beta)+kron(diag(ones(1,Np-1),-1),beta');end

ii=0;for EE=[-0.05:1e-2:1.05]*t0
ii=ii+1;ig0=(EE+zplus)*eye(NW)-alpha;
if ii==1
gs1=inv(ig0);gs2=inv(ig0);end
change=1;
while change > 1e-6
Gs=inv(ig0-beta'*gs1*beta);
change=sum(sum(abs(Gs-gs1)))/(sum(sum(abs(gs1)+abs(Gs))));
gs1=0.5*Gs+0.5*gs1;
end
sig1=beta'*gs1*beta;sig1=kron(L,sig1);gam1=i*(sig1-sig1');

change=1;
while change > 1e-6
Gs=inv(ig0-beta'*gs2*beta');
change=sum(sum(abs(Gs-gs2)))/(sum(sum(abs(gs2)+abs(Gs))));
gs2=0.5*Gs+0.5*gs2;
end
```



```

sig2=beta*gs2*beta';sig2=kron(R,sig2);gam2=i*(sig2-sig2');

G=inv((EE*eye(Np*NW))-H-sig1-sig2);
DD=real(diag(i*(G-G')))/2/pi;
Tcoh(ii)=real(trace(gam1*G*gam2*G'));E(ii)=EE/t0;ii
end

ii=1;for kk=pi*[-1:0.01:1]
H=alpha+beta*exp(i*kk)+beta'*exp(-i*kk);
[V,D]=eig(H);EK(:,ii)=sort(abs(diag(D)))/t0;K(ii)=kk/pi;ii=ii+1;
end

X=linspace(0,9,101);Ean= 2*(1-cos(pi*X/(NW+1)));
hold on
figure(1)
h=plot(Tcoh,E,'k');
set(h,'linewidth',[3.0])
%h=plot(X,Ean,'k--');
%set(h,'linewidth',[1.2])
set(gca,'FontSize',[36])
axis([0 10 -.1 1])

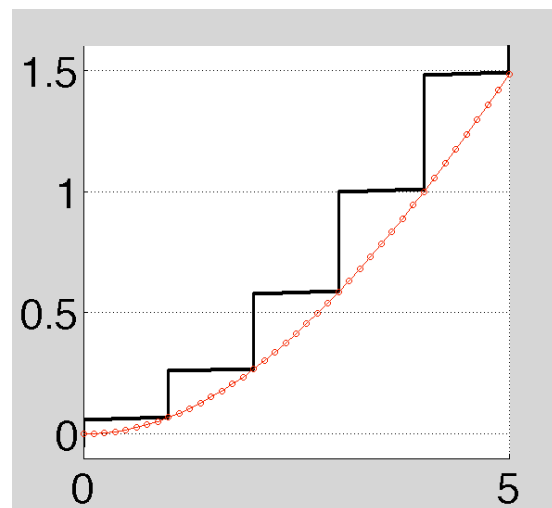
```

- (a) Write a code to calculate the transmission for a ballistic conductor with 11 points along the width.
- (b) Use this code to locate the energies at which the first three steps occur and compare with an appropriate analytical expression.

### SOLUTION:

Change NW to 11: Steps match analytical expression (red curve) very well.

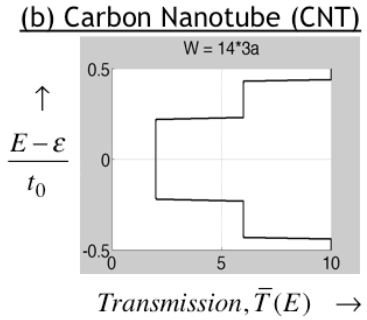
$$E_{an} = 2 \cdot (1 - \cos(\pi \cdot n / (NW + 1)))$$



**TH7: Graphene or CNT**

Fig.21.3b in LNE shows the transmission versus energy for a zigzag carbon nanotube obtained with the code given below:

Fig.21.3b →



```
clear all
%Constants (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;qh=q/hbar;a=1e-9;

%inputs

t0=-2.5;D=1e-50;ctr=0;zplus=i*1e-3;
NL=1;L=zeros(NL);R=L;L(1,1)=1;R(NL,NL)=1;
config=2;%1 for armchair, 2 for zigzag edge
% NW=floor(14*sqrt(3));% Armchair
NW=14;% Zigzag

%Hamiltonian
al=t0*[0 1 0 0;1 0 1 0;0 1 0 1;0 0 1 0];
if config==1
bL=t0*[0 0 0 0;0 0 0 0;0 0 0 0;1 0 0 0];
bW=t0*[0 0 0 0;1 0 0 0;0 0 0 1;0 0 0 0];end
if config==2
bW=t0*[0 0 0 0;0 0 0 0;0 0 0 0;1 0 0 0];
bL=t0*[0 0 0 0;1 0 0 0;0 0 0 1;0 0 0 0];end

n=4;
alpha=kron(eye(NW),al)+kron(diag(ones(1,NW-1),+1),bW)+kron(diag(ones(1,NW-1),-1),bW');
alpha=alpha+kron(diag(ones(1,1),1-NW),bW)+kron(diag(ones(1,1),NW-1),bW');% for CNT's

ii=0;for EE=t0*[-0.5:+0.01:+0.5]
ii=ii+1;
ig0=(EE+zplus)*eye(NW*n)-alpha;
if ii==1
gs1=inv(ig0);gs2=inv(ig0);end

BB=0;beta=kron(diag(exp(i*qh*BB*a*a*[1:1:NW])),bL);
%beta=kron(eye(NW),bL);
H=kron(eye(NL),alpha);if NL>1
```

```

H=H+kron(diag(ones(1,NL-1),+1),beta)+...
kron(diag(ones(1,NL-1),-1),beta');end

change=1;
while change>1e-4
    Gs=inv(ig0-beta'*gs1*beta);
    change=sum(sum(abs(Gs-gs1)))/(sum(sum(abs(gs1)+abs(Gs))));
    gs1=0.5*Gs+0.5*gs1;
end
sig1=beta'*gs1*beta;sig1=kron(L,sig1);gam1=i*(sig1-sig1');
change=1;
while change>1e-4
    Gs=inv(ig0-beta*gs2*beta');
    change=sum(sum(abs(Gs-gs2)))/(sum(sum(abs(gs2)+abs(Gs))));
    gs2=0.5*Gs+0.5*gs2;
end
sig2=beta*gs2*beta';sig2=kron(R,sig2);gam2=i*(sig2-sig2');

G=inv((EE*eye(NW*NL*n))-H-sig1-sig2);
T(ii)=real(trace(gam1*G*gam2*G'));E(ii)=EE/t0;
if EE==0
    T(ii)=T(ii-1);end,EE
end

hold on
h=plot(T,E,'k');
set(h,'linewidth',[3.0])
set(gca,'FontSize',[36]);
axis([0 10 -0.5 +0.5])
title(' W = 14 * 3a ')
grid on

```

- (a) Write your own code to reproduce Fig.21.3b.
- (b) Compare the energies at which the steps occur with an appropriate analytical expression.

**SOLUTION:**

$$E = \hbar v_0 k \quad \text{at } k$$

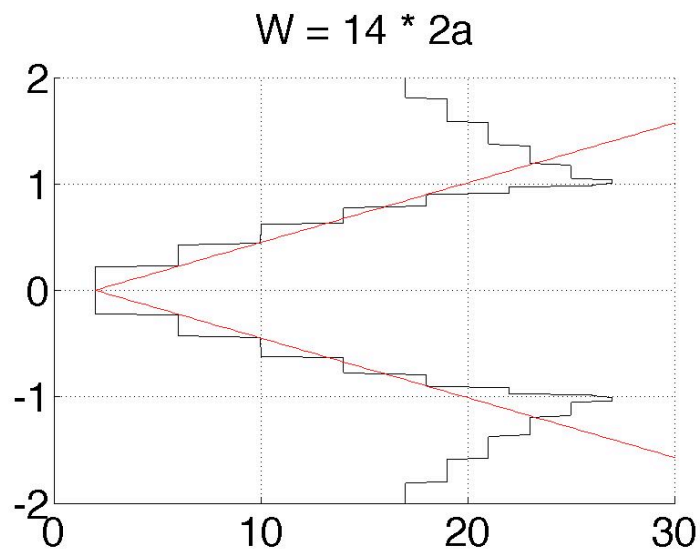
$$k = \frac{2(\text{forPBC}) * n \pi}{NW * 2a}$$

$$\frac{E}{t} = a \frac{2n\pi}{NW * 2a} \rightarrow n = \frac{E}{t} * \frac{2 * NW}{2\pi}$$

$$M = 4n + 2 = \frac{E}{t} * \frac{4 * NW}{\pi} + 2$$

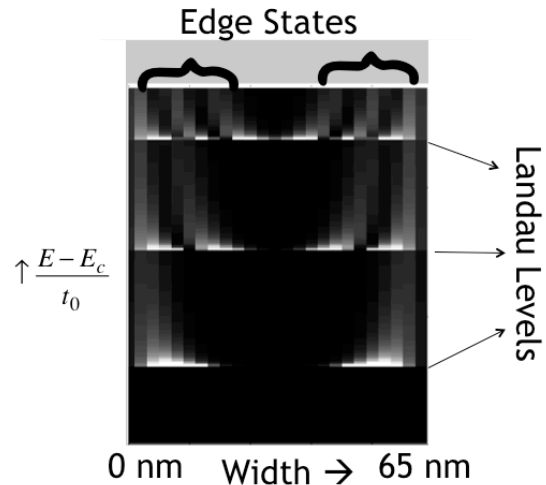
*Matches well near  $E = 0$ , but not at energies far from  $E = 0$ , because we are using an approximate dispersion relation*

$$E = \hbar v_0 k \quad \text{at } k$$



### TH8: Quantum Hall effect

Fig.21.4 of LNE shows the Hall resistance as a function of the B-field with the famous quantum Hall plateaus clearly evident. These plateaus can be understood in terms of the formation of edge states evident from the local density of states plot in Fig.21.5 for a magnetic field of  $B=20\text{T}$ .



Below is my code used to calculate Fig.21.5.

```
clear all
%Constants (all MKS, except energy which is in eV)
hbar=1.06e-34;q=1.6e-19;m=0.1*9.1e-31;qh=q/hbar;B=20;

%inputs
a=2.5e-9;t0=(hbar^2)/(2*m*(a^2)*q);
NW=25;Np=1;L=zeros(Np);R=L;L(1,1)=1;R(Np,Np)=1;zplus=i*1e-12;

%Hamiltonian
al=4*t0;by=-t0;bx=-t0;
alpha=kron(eye(NW),al)+kron(diag(ones(1,NW-1),+1),by)+kron(diag(ones(1,NW-1),-1),by');
alpha=alpha+diag([1:1:NW].*0);
beta=kron(diag(exp(i*qh*B*a*a*[1:1:NW])),bx);
H=kron(eye(Np),alpha);
if Np>1
H=H+kron(diag(ones(1,Np-1),+1),beta)+kron(diag(ones(1,Np-1),-1),beta');end

ii=0;for EE=[-0.05:0.008:1.05]*t0
ii=ii+1;ig0=(EE+zplus)*eye(NW)-alpha;
if ii==1
gs1=inv(ig0);gs2=inv(ig0);end
change=1;
while change>1e-4
Gs=inv(ig0-beta'*gs1*beta);
change=sum(sum(abs(Gs-gs1)))/(sum(sum(abs(gs1)+abs(Gs))));
gs1=0.5*Gs+0.5*gs1;
end
sig1=beta'*gs1*beta;sig1=kron(L,sig1);gam1=i*(sig1-sig1');

change=1;
while change>1e-4
```

```

Gs=inv(ig0-beta*gs2*beta');
change=sum(sum(abs(Gs-gs2)))/(sum(sum(abs(gs2)+abs(Gs))));
gs2=0.5*Gs+0.5*gs2;
end
sig2=beta*gs2*beta';sig2=kron(R,sig2);gam2=i*(sig2-sig2');

G=inv((EE*eye(Np*NW))-H-sig1-sig2);
DD(:,ii)=real(diag(i*(G-G')))./2/pi;
Gn=G*gam1*G';
NN(:,ii)=real(diag(Gn))./2/pi;
end

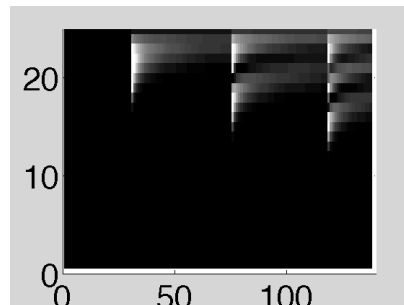
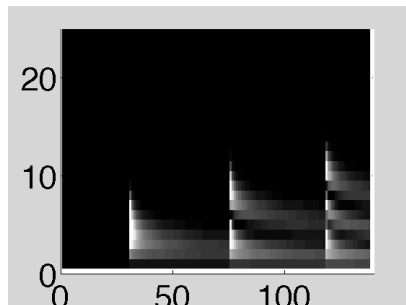
XX=DD;
lo=.4*min(min(XX));hi=.4*max(max(XX));

figure(1)
hold on
imagesc(XX,[lo hi])
colormap(gray)
set(gca,'FontSize',[36])
grid on
axis([0 140 0 25])

```

- (a) Write a code to reproduce the plot of the local density of states shown in Fig.21.5.
- (b) Use your code to plot the local electron density assuming  $f_1 = 1$ ,  $f_2 = 0$ .
- (c) Use your code to plot the local electron density assuming  $f_1 = 0$ ,  $f_2 = 1$ .  
Change  $G_n = G * \text{gam1} * G'$  to  $G_n = G * \text{gam2} * G'$
- (d) Explain why (b) and (c) look so different.

### SOLUTION:



*In one case electrons come in from the left and are pushed to one side of the sample by the magnetic field while in the other case they come in from the right and are pushed to the other side.*

**TH9: Non-local spin voltage**

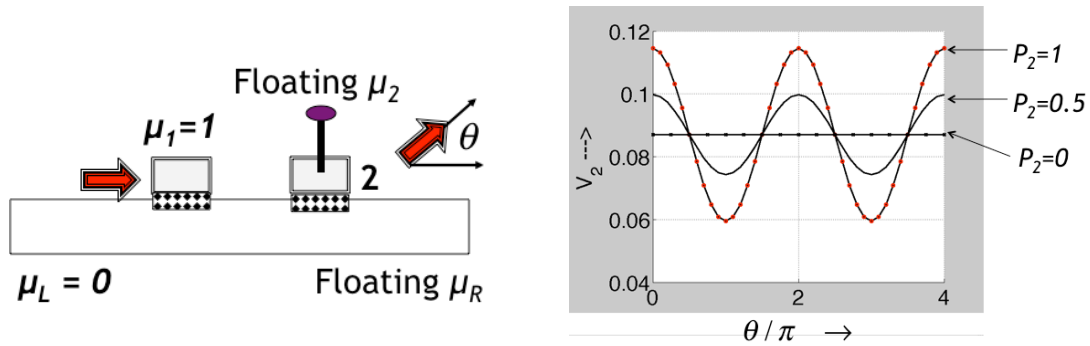


Fig.22.6 in LNE shows the non-local spin voltage outside the current path calculated using the code given below:

```
clear all
hbar=1.06e-34;q=1.6e-19;m=0.1*9.1e-31;a=2.5e-
9;t0=(hbar^2)/(2*m*(a^2)*q);
sx=[0 1;1 0];sy=[0 -i;i 0];sz=[1 0;0 -1];zplus=1i*1e-12;

Np=50;N1=10;N2=20;X=1*[0:1:Np-1];
L=diag([1 zeros(1,Np-1)]);
R=diag([zeros(1,Np-1) 1]);
L1=0.1*diag([zeros(1,N1-1) 1 zeros(1,Np-N1)]);
L2=0.1*diag([zeros(1,N2-1) 1 zeros(1,Np-N2)]);

ii=0;for theta=[0:0.1:4]*pi
    P1=0.7*[0 0 1];
    P2=1*[sin(theta) 0 cos(theta)];ii=ii+1;

H0=diag(ones(1,Np));
HR=diag(ones(1,Np-1),1);HL=diag(ones(1,Np-1),-1);

H=2*t0*kron(H0,eye(2))-t0*kron(HL,eye(2))-t0*kron(HR,eye(2));

EE=t0;ck=(1-(EE+zplus)/(2*t0));ka=acos(ck);
sL=-t0*exp(1i*ka)*eye(2);sR=sL;
s1=-t0*exp(1i*ka)*(eye(2)+P1(1)*sx+P1(2)*sy+P1(3)*sz);
s2=-t0*exp(1i*ka)*(eye(2)+P2(1)*sx+P2(2)*sy+P2(3)*sz);
```

```

sigL=kron(L,sL);sigR=kron(R,sR);
sig1=kron(L1,s1);sig2=kron(L2,s2);
gamL=1i*(sigL-sigL');gamR=1i*(sigR-sigR');
gam1=1i*(sig1-sig1');gam2=1i*(sig2-sig2');

G=inv(((EE+zplus)*eye(2*Np))-H-sigL-sigR-sig1-sig2);

% {1 L} {2 R} = {a} {b}

TM1L=real(trace(gam1*G*gamL*G'));
TML1=real(trace(gamL*G*gam1*G'));
Taa=[0 TM1L;TML1 0];

TM12=real(trace(gam1*G*gam2*G'));
TM1R=real(trace(gam1*G*gamR*G'));
TML2=real(trace(gamL*G*gam2*G'));
TMLR=real(trace(gamL*G*gamR*G'));
Tab=[TM12 TM1R;TML2 TMLR];

TM21=real(trace(gam2*G*gam1*G'));
TM2L=real(trace(gam2*G*gamL*G'));
TMR1=real(trace(gamR*G*gam1*G'));
TMRL=real(trace(gamR*G*gamL*G'));
Tba=[TM21 TM2L;TMR1 TMRL];

TM2R=real(trace(gam2*G*gamR*G'));
TMR2=real(trace(gamR*G*gam2*G'));
Tbb=[0 TM2R;TMR2 0];

Taa=diag(sum(Taa)+sum(Tba))-Taa;Tba=-Tba;
Tbb=diag(sum(Tab)+sum(Tbb))-Tbb;Tab=-Tab;
if abs(sum(sum([Taa Tab;Tba Tbb]))) > 1e-10
    junk=100,end

V=-inv(Tbb)*Tba*[1;0];
VV2(ii)=V(1);VVR(ii)=V(2);
angle(ii)=theta/pi;
I2(ii)=TM21;IL(ii)=TML1;IR(ii)=TMR1;

Gn=G*(gam1+V(1)*gam2+V(2)*gamR)*G';
Gn=Gn([2*N2-1:2*N2],[2*N2-1:2*N2]);
A=i*(G-G');A=A([2*N2-1:2*N2],[2*N2-1:2*N2]);
g2=i*(s2-s2');XX2(ii)=real(trace(g2*Gn)/trace(g2*A));
end
X2=VV2;XR=VVR;max(X2)-min(X2)

```



```

hold on
h=plot(angle,X2,'k');
set(h,'linewidth',2.0)
h=plot(angle,XX2,'ro');
set(h,'linewidth',2.0)
set(gca,'FontSize',36)
xlabel(' \theta / \pi ---> ')
ylabel(' V_{2} ---> ')
grid on

```

(a) Write a code to reproduce Fig.22.6.

(b) Note that a significant fraction of this code is devoted to solving the Buttiker equations for a four-terminal structure with voltages applied to two terminals while the other two terminals are left floating. Explain how this is done.

(c)

**SOLUTION:**

$$I_i = \sum_j T_{ij} (f_i - f_j) \rightarrow \begin{Bmatrix} I_1 \\ I_L \\ I_2 \\ I_R \end{Bmatrix} = \begin{bmatrix} T_{aa} & T_{ab} \\ T_{ba} & T_{bb} \end{bmatrix} \begin{Bmatrix} f_1 \\ f_L \\ f_2 \\ f_R \end{Bmatrix}$$

$$T_{aa} = \begin{bmatrix} T_{1L} + T_{12} + T_{1R} & -T_{1L} \\ -T_{L1} & T_{L1} + T_{L2} + T_{LR} \end{bmatrix}$$

$$T_{ab} = \begin{bmatrix} -T_{12} & -T_{1R} \\ -T_{L2} & -T_{LR} \end{bmatrix} \quad T_{ba} = \begin{bmatrix} -T_{21} & -T_{2L} \\ -T_{R1} & -T_{RL} \end{bmatrix}$$

$$T_{bb} = \begin{bmatrix} T_{2L} + T_{21} + T_{2R} & -T_{2R} \\ -T_{R2} & T_{R1} + T_{R2} + T_{RL} \end{bmatrix}$$

$$\begin{Bmatrix} I_2 \\ I_R \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} = T_{ba} \begin{Bmatrix} f_1 \\ f_L \end{Bmatrix} + T_{bb} \begin{Bmatrix} f_2 \\ f_R \end{Bmatrix}$$

$$\rightarrow \begin{Bmatrix} f_2 \\ f_R \end{Bmatrix} = -T_{bb}^{-1} T_{ba} \begin{Bmatrix} f_1 \\ f_L \end{Bmatrix} = -T_{bb}^{-1} T_{ba} \begin{Bmatrix} 1 \\ 0 \end{Bmatrix}$$

***TH10: Voltage controlled spin precession (“Spin transistor”)***

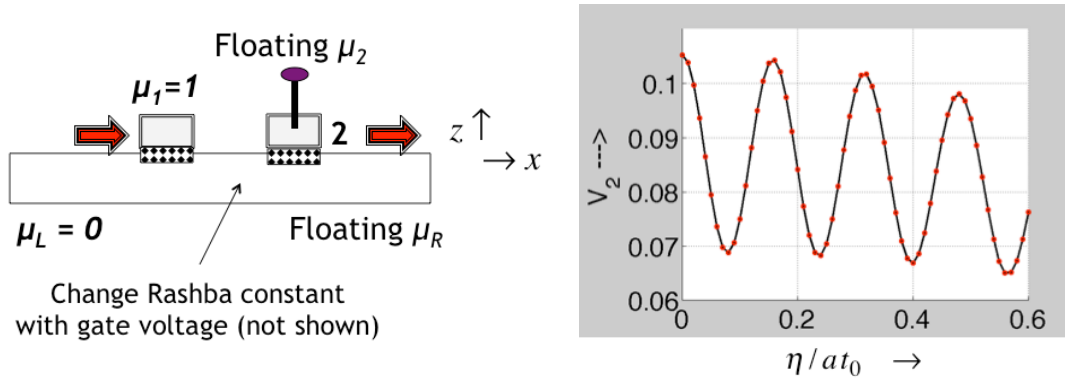


Fig.22.7 in LNE shows the modulation in the output voltage as a function of the Rashba spin-orbit coupling coefficient which can be changed through a gate voltage. Below is my code showing this effect:

```
clear all
hbar=1.06e-34;q=1.6e-19;m=0.1*9.1e-31;a=2.5e-
9;t0=(hbar^2)/(2*m*(a^2)*q);
sx=[0 1;1 0];sy=[0 -1i;1i 0];sz=[1 0;0 -1];zplus=1i*1e-12;

Np=50;N1=5;N2=45;X=1*[0:1:Np-1];
L=diag([1 zeros(1,Np-1)]);
R=diag([zeros(1,Np-1) 1]);

L1=0.1*diag([zeros(1,N1-1) 1 zeros(1,Np-N1)]);
L2=0.1*diag([zeros(1,N2-1) 1 zeros(1,Np-N2)]);

ii=0;for al=[0:0.005:0.3]*t0
    P1=[0 0 0.7];P2=[0 0 0.7];ii=ii+1;
    alph=al*1;% Rashba
    BB=al*0;% Hanle

    H0=diag(ones(1,Np));
    HR=diag(ones(1,Np-1),1);HL=diag(ones(1,Np-1),-1);
    beta=t0*eye(2)+1*i*alph*sy;
    alpha=2*t0*eye(2)+1*BB*sy;

    H=kron(H0,alpha)-kron(HL,beta')-kron(HR,beta);

    EE=t0;ck=(1-(EE+zplus)/(2*t0));ka=acos(ck);
    sL=-t0*exp(1i*ka)*eye(2);sR=sL;
    s1=-t0*exp(1i*ka)*(eye(2)+P1(1)*sx+P1(2)*sy+P1(3)*sz);
```

```

s2=-t0*exp(1i*ka)*(eye(2)+P2(1)*sx+P2(2)*sy+P2(3)*sz);

sigL=kron(L,sL);sigR=kron(R,sR);
sig1=kron(L1,s1);sig2=kron(L2,s2);
gamL=1i*(sigL-sigL');gamR=1i*(sigR-sigR');
gam1=1i*(sig1-sig1');gam2=1i*(sig2-sig2');

G=inv(((EE+zplus)*eye(2*Np))-H-sigL-sigR-sig1-sig2);

% {1 L} {2 R} = {a} {b}
TM1L=real(trace(gam1*G*gamL*G'));
TML1=real(trace(gamL*G*gam1*G'));
Taa=[0 TM1L;TML1 0];

TM12=real(trace(gam1*G*gam2*G'));
TM1R=real(trace(gam1*G*gamR*G'));
TML2=real(trace(gamL*G*gam2*G'));
TMLR=real(trace(gamL*G*gamR*G'));
Tab=[TM12 TM1R;TML2 TMLR];

TM21=real(trace(gam2*G*gam1*G'));
TM2L=real(trace(gam2*G*gamL*G'));
TMR1=real(trace(gamR*G*gam1*G'));
TMRL=real(trace(gamR*G*gamL*G'));
Tba=[TM21 TM2L;TMR1 TMRL];

TM2R=real(trace(gam2*G*gamR*G'));
TMR2=real(trace(gamR*G*gam2*G'));
Tbb=[0 TM2R;TMR2 0];

Taa=diag(sum(Taa)+sum(Tba))-Taa;Tba=-Tba;
Tbb=diag(sum(Tab)+sum(Tbb))-Tbb;Tab=-Tab;
if abs(sum(sum([Taa Tab;Tba Tbb]))) > 1e-10
    junk=100,end

V=-inv(Tbb)*Tba*[1;0];
VV2(ii)=V(1);VVR(ii)=V(2);
alp(ii)=al*2/t0;% eta/t0/a

Gn=G*(gam1+V(1)*gam2+V(2)*gamR)*G';A=i*(G-G');
VV(ii)=real(trace(gam2*Gn)/trace(gam2*A));
end

hold on
h=plot(alp,VV2,'k');
set(h,'linewidth',2.0)

```

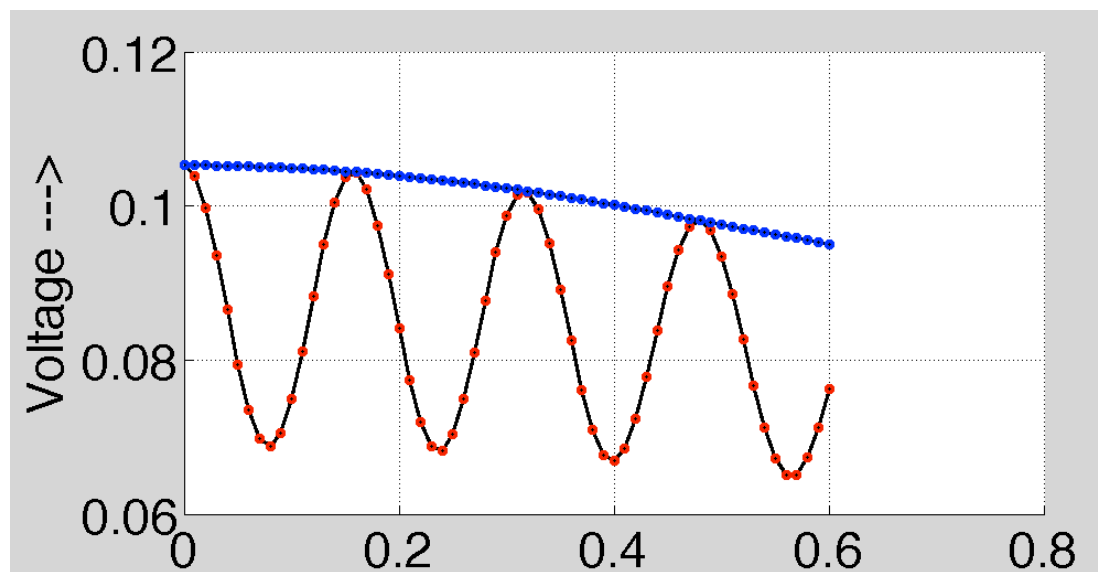
```

h=plot(alp,VV,'ro');
set(h,'linewidth',2.0)
set(gca,'FontSize',36)
ylabel(' Voltage ---> ')
grid on

```

- (a) Write a code to reproduce Fig.22.7 with contacts 1 and 2 both polarized along z.
- (b) Obtain the same plot assuming that contacts 1 and 2 are both polarized along x.
- (c) Obtain the same plot assuming that contacts 1 and 2 are both polarized along y.
- (d) Compare your results in (a), (b) and (c) and explain physically why two of these look similar and one looks very different.

### SOLUTION:



(a) and (b) give red curve, while (c) gives blue curve.

The difference because electrons traveling along x feel an effective magnetic field along y and precess around it. In (a) and (b) electrons are polarized along z and x and show modulation due to this precession around y. But in (c) electrons are polarized along y and do not precess.