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Quantum Transport: Atom to Transistor

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Solutions to non-Matlab Exercises

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E.2.3. $\frac{\partial \Psi}{\partial x} = \left(\gamma e^{\gamma x} - \gamma a e^{-\gamma x}\right) e^{-iEt/\hbar}$

$$\Psi^* \frac{\partial \Psi}{\partial x} = \left(e^{\gamma^* x} + a^* e^{-\gamma^* x}\right)\left(\gamma e^{\gamma x} - \gamma a e^{-\gamma x}\right)$$

$$= \gamma e^{(\gamma+\gamma^*)x} - \gamma |a|^2 e^{-(\gamma+\gamma^*)x}$$

$$- \gamma a\, e^{-(\gamma-\gamma^*)x} + \gamma a^*\, e^{(\gamma-\gamma^*)x}$$

$$J = \frac{\hbar}{m} \mathrm{Im}\left(\Psi^* \frac{\partial \Psi}{\partial x}\right)$$

(a) If $\gamma = i\beta$ with real β,

$$J = \frac{\hbar\beta}{m}\left(1 - |a|^2\right)$$

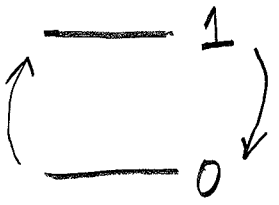
(b) If γ is real,

$$J = \frac{\hbar\gamma}{m} \mathrm{Im}\left(a^* - a\right)$$

$$= \frac{2\hbar\gamma}{m} \mathrm{Im}(a)$$

E.3.4.

$$\frac{dP_1}{dt} = -\frac{dP_0}{dt} = 0$$ (at steady-state)



$$= P_0\left[\frac{\gamma_1 f_1 + \gamma_2 f_2}{\hbar}\right] - P_1\left[\frac{\gamma_1(1-f_1) + \gamma_2(1-f_2)}{\hbar}\right]$$

$$\frac{P_1}{P_0} = \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1(1-f_1) + \gamma_2(1-f_2)}$$

Hence, $$\frac{P_1}{P_1 + P_0} = P_1 = \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}$$

$$N = \sum_n n P_n = P_1$$

$$I = q\left(P_0 \frac{\gamma_1 f_1}{\hbar} - P_1 \frac{\gamma_1(1-f_1)}{\hbar}\right)$$

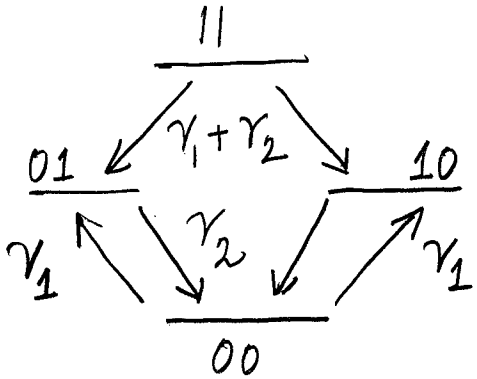
$$= \frac{q\gamma_1}{\hbar}(f_1 - P_1) = \frac{q\gamma_1\gamma_2}{\hbar(\gamma_1+\gamma_2)}(f_1 - f_2)$$

E.3.6. Can assume $P_{01} = P_{10}$ due to symmetry

(a) $f_1'' = 0$

$f_2' = f_2'' = 0$

$f_1' = 1$



MATLAB codes used to generate text figures

Chapter 1

% Fig.1.1.1

```
clear all

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

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

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

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

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

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

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

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

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

% Fig.1.1.3

```
clear all

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

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

% Fig.1.3.3, 1.5.1

```
clear all

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

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

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

% Fig.1.4.6

```
clear all

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

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

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

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

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

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