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% spinNEGF1D
% 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
sx=[0 1;1 0];sy=[0 -i;i 0];sz=[1 0;0 -1];B=0;
[vx,dd]=eig(sx);[vy,dd]=eig(sy);[vz,dd]=eig(sz);
V=vz;dn=V*[1 0;0 0]*V';up=V*[0 0;0 1]*V';
%%
% dn=1/2*(eye(2)+sx);up=1/2*(eye(2)-sx);
%%

% Inputs
hbar=1.06e-34;q=1.6e-19;m=0.03*9.1e-31;
a=1e-9;t0=(hbar^2)/(2*m*(a^2)*q);
zplus=i*1e-12;

Np=51;L=zeros(Np);R=L;L(1,1)=1;R(Np,Np)=1;
ctr=0;D=1e-5*kron(eye(Np),ones(2));

sigB=zeros(2*Np);siginB=zeros(2*Np);

ii=1;for EE=0.2:1:0.2
    for rashba=-1e-10:1e-12:1e-10
        alpha=2*t0*eye(2);beta=-t0*eye(2)+(rashba/i/2/a)*sy;
        H=kron(eye(Np),alpha)+kron(diag(ones(1,Np-1),+1),beta)+...
            kron(diag(ones(1,Np-1),-1),beta');

        ck=(1-(EE+zplus)/(2*t0));ka=acos(ck);
        sigu=(-t0*exp(i*ka))*up;sigd=(-t0*exp(i*ka))*dn;
        sig1u=kron(L,sigu);sig1d=kron(L,sigd);
        sig2u=kron(R,sigu);sig2d=kron(R,sigd);
        gam1u=i*(sig1u-sig1u');gam1d=i*(sig1d-sig1d');
        gam2u=i*(sig2u-sig2u');gam2d=i*(sig2d-sig2d');

        change=1;
        while change>5e-8
            G=inv((EE*eye(2*Np))-H-sig1u-sig1d-sig2u-sig2d-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-8
            Gn=G*(gam1u+siginB)*G';
            siginBnew=D.*Gn;
            change=ctr*(sum(sum(abs(siginBnew-siginB))))/(sum(sum(abs(siginBnew+siginB))));

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    siginB=siginB+0.25*ctr*(siginBnew-siginB);
end
TM(ii)=real(trace(gam2u*Gn));
TMd(ii)=real(trace(gam2d*Gn));
Ttest(ii)=real(trace(gam1u*G*gam2d*G'));
E(ii)=EE;X(ii)=rashba;ii=ii+1
end
end

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%%  

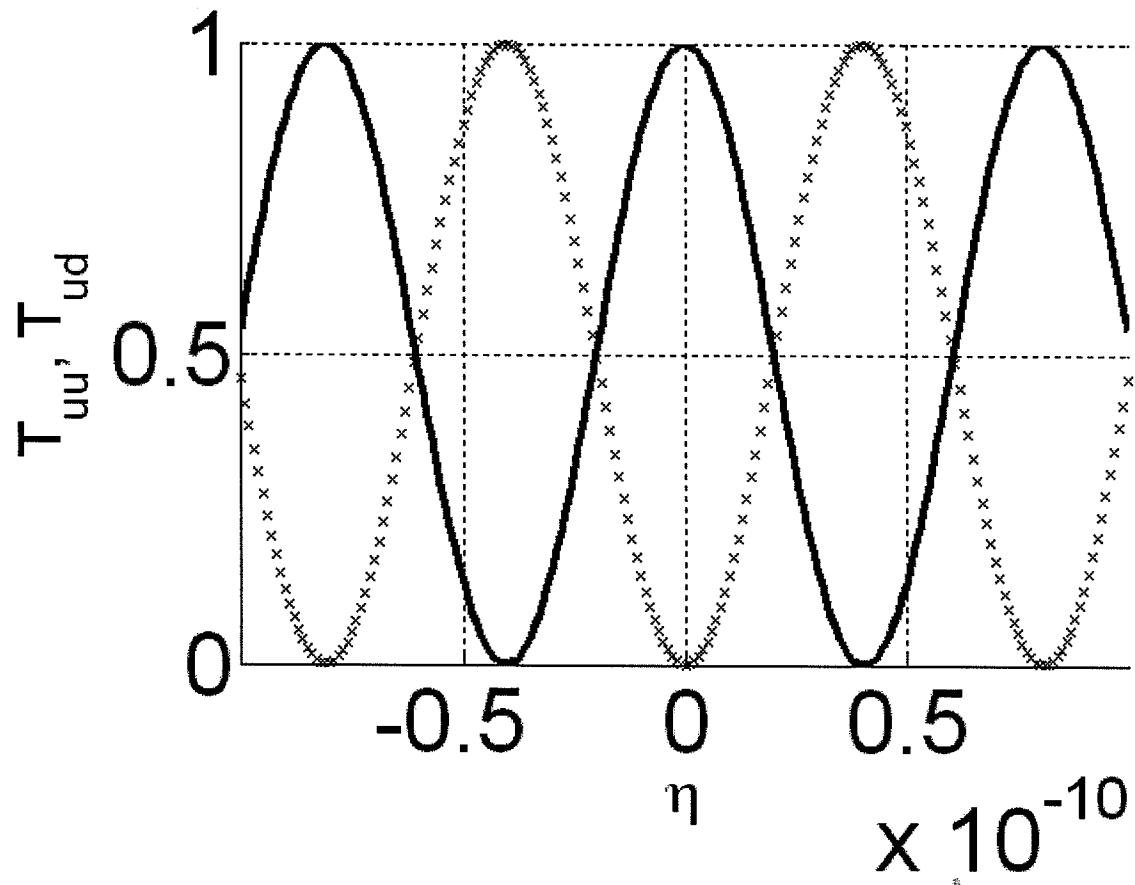
pi*hbar^2/m/(a*(Np-1))/q

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hold on
h=plot(X,TM,'r');
set(h,'linewidth',[3.0])
h=plot(X,TMd,'bx');
set(gca,'Fontsize',[36])
h=plot(X,Ttest,'yo');
grid on

```



**Analytical value = 8.0813e-011**

### Problem 1 (b) /

$$H_{SO} = \frac{e}{2} k_x \nabla_y \equiv M_B \nabla_y B_y$$

(From  $M_B \vec{\nabla} \cdot \vec{B}$ )

$$\therefore B_y = \frac{e k_x}{M_B} \quad (\text{effective magnetic field})$$

$$\frac{d\vec{S}}{dt} = \frac{2M_B}{\hbar} (\vec{B} \times \vec{S})$$

If  $\vec{S}$  is not along the  $\vec{B}$  direction, then  $\vec{S}$  will rotate. For example in this problem,  $\vec{B} = B_y \hat{y}$  and if  $\vec{S}$  is along  $\hat{x}$  or  $\hat{z}$  direction  $\vec{S}$  will rotate with angular speed  $= \frac{2M_B B}{\hbar}$

$$\phi = \frac{2M_B B}{\hbar} t$$

$$= \frac{2e k_x}{\hbar} \frac{L m^*}{\hbar k_x}$$

$$= \frac{2m^* L e}{\hbar^2} \quad (= 2\pi \text{ for } \zeta_p)$$

$$\zeta_p = \frac{\pi \hbar^2}{m^* L} \simeq 0.81 \times 10^{-10} [\text{eV} \cdot \text{m}]$$

$$\begin{cases} m^* = 0.03 \times 9.1 \times 10^{-31} \text{ kg} \\ \hbar = 1.06 \times 10^{-34} \text{ J} \cdot \text{s} \\ L = 100 \text{ nm} \end{cases}$$

Another approach /

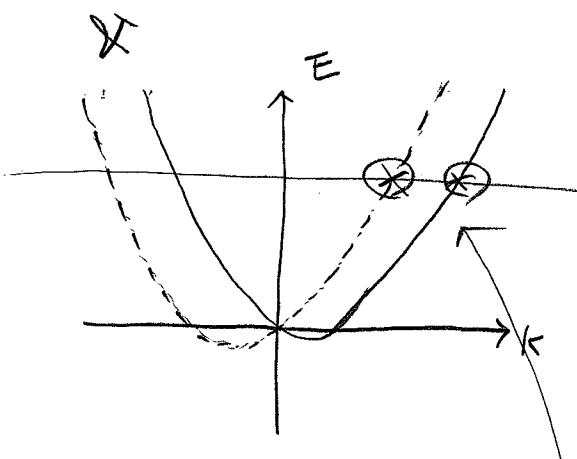
Let's say Injecting spin is  $+z$  polarized  $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ .

With Rashba term, Hamiltonian would be

$$H = \begin{bmatrix} \frac{\hbar^2 k^2}{2m} & \gamma(-ik) \\ \gamma ik & \frac{\hbar^2 k^2}{2m} \end{bmatrix}$$

$$E(k) = \frac{\hbar^2 k^2}{2m} \pm \gamma k$$

$$\text{basis} \Rightarrow \frac{1}{\sqrt{2}} \left\{ \begin{pmatrix} 1 \\ i \end{pmatrix}, \begin{pmatrix} 1 \\ -i \end{pmatrix} \right\}$$



At same energy, there will be two different  $k$  values.

$$E = \frac{\hbar^2 k_1^2}{2m} + \gamma k_1 = \frac{\hbar^2 k_2^2}{2m} - \gamma k_2 \quad (*)$$

As each state goes through the device, it will pick up distinct phase.

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 \\ i \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

Let's assume device length is  $L$ .

$$\frac{1}{2} e^{ik_1 L} \begin{pmatrix} 1 \\ i \end{pmatrix} + \frac{1}{2} e^{ik_2 L} \begin{pmatrix} 1 \\ -i \end{pmatrix} = \begin{pmatrix} \cos \frac{\Delta k L}{2} \\ -\sin \frac{\Delta k L}{2} \end{pmatrix} e^{i k_0 L}$$

$$\left( k_0 = \frac{k_1 + k_2}{2}, \Delta k = k_1 - k_2 \right)$$

From (\*),  $\frac{\hbar^2}{2m^*} (k_1^2 - k_2^2) = \frac{e}{2} (k_1 + k_2)$

$$k_1 - k_2 = \Delta k = \frac{2m^* \frac{e}{2}}{\hbar^2}$$

$$\therefore \theta = \Delta k L = \frac{2m^* \frac{e}{2} L}{\hbar^2} \quad (\text{Same result})$$

Problem 2 (a) /

$$\begin{cases} \nabla_a \nabla_b - \nabla_b \nabla_a = 2i \sum_c \epsilon_{abc} \nabla_c \\ \nabla_a \nabla_b + \nabla_b \nabla_a = 2\delta_{ab} I \end{cases}$$

$$\therefore \nabla_i \nabla_j = f_{ij} I + i \sum_k \epsilon_{ijk} \nabla_k$$

$$[\vec{\nabla}, \vec{C}] [\vec{\nabla}, \vec{D}]$$

$$= \sum_{ij} \nabla_i C_i \nabla_j D_j$$

$$= \sum_{ij} C_i D_j [ f_{ij} I + i \sum_k \epsilon_{ijk} \nabla_k ]$$

$$= \sum_i C_i D_i I + i \sum_k \nabla_k \sum_{ij} \epsilon_{ijk} C_i D_j$$

$$= (\vec{C} \cdot \vec{D}) I + i \vec{\nabla} \cdot (\vec{C} \times \vec{D})$$

$$(b) (\vec{\nabla} \cdot (\vec{P} + q\vec{A})) (\vec{\nabla} \cdot (\vec{P} + q\vec{A}))$$

$$= (\vec{P} + q\vec{A}) \cdot (\vec{P} + q\vec{A}) I + i \vec{\nabla} \cdot (\vec{P} + q\vec{A}) \times (\vec{P} + q\vec{A})$$

$$= (\vec{P} + q\vec{A}) \times (\vec{P} + q\vec{A}) \{4\}$$

$$= (\vec{P} \times \vec{P} + q^2 \vec{A} \times \vec{A}^\perp + \vec{P} \times q\vec{A} + q\vec{A} \times \vec{P}) \{4\}$$

$$(\vec{P} \times \vec{P}) \{4\} = 0 \quad \because (\vec{P} \times \vec{P}) \{4\} = (P_x P_y - P_y P_x) \{4\} = 0$$

$$\begin{aligned}
 & (\vec{p} \times \vec{A} + \vec{A} \times \vec{p}) \{4\} \\
 = & -ik (\nabla \times (\vec{A} \psi) + \vec{A} \times (\nabla \psi)) \\
 = & -ik (\psi (\nabla \times \vec{A}) + (\nabla \psi) \times \vec{A} + \vec{A} \times (\nabla \psi)) \\
 = & -ik (\vec{B} \psi + \vec{A} \times (\nabla \psi) - \vec{A} \times (\nabla \psi)) \\
 = & -ik \vec{B} \{4\}
 \end{aligned}$$

Collecting all terms gives

$$\begin{aligned}
 & (\vec{\nabla} \cdot (\vec{p} + q\vec{A})) (\vec{\nabla} \cdot (\vec{p} + q\vec{A})) \{4\} \\
 = & (\vec{p} + q\vec{A}) \cdot (\vec{p} + q\vec{A}) \{4\} + ik \cdot (-ik q \vec{B}) \{4\} \\
 = & (\vec{p} + q\vec{A}) \cdot (\vec{p} + q\vec{A}) \{4\} + qk \vec{\nabla} \cdot \vec{B} \{4\}
 \end{aligned}$$