

Supplement QM
Multilayer Quantum Well-and-Barrier Analysis Software Program

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I. INTRODUCTION

Supplement QM. This supplement contains the listings of all the Matlab .m files used in determining the reflectance and transmittance characteristics of multilayer quantum well-and-barrier structures. In addition, there are files for displaying graphical results. A number of Matlab script .m files contain examples of various multilayer quantum well-and-barrier structures.

II. MAIN PROGRAM

The main program, called AQM.m, is the first program in the listing.

AQM.m

```
% MAIN PROGRAM NAME: AQM
% Step 1: Specify Initial Quantities
clear; clf; clc; Prelim; Structure;
% Step 2: Draw Quantum Well and Barrier Structure
[L] = DrawMQW(PotentP,PotentQ,PotentF,ThickP,ThickQ,ThickF,DS,CG);
% Step 3: Vary the Vacuum Energy
for E = EnergyMin:EnergyDel:EnergyMax
E = E + Eo;
% Step 4: Convert EM Quantities to QM Quantities
Convert;
% Step 5: Compute TE and TM Incident Wavefunctions
[PsiI_TE,PsiI_TM] = PsiI(ThetaI,epP,muP);
% Step 6: Region P, Q, and F Calculations
RegionP; RegionQ; RegionF;
% Step 7: Compute Thin-Film Phases and Matrix Q
Phases; MatrixQ;
% Step 8: Compute the Matrices MR AND MT
[MR,MT] = MatrixMRMT(Q);
% Step 9: Compute Reflectance and Transmittance
Wavefunction; Probability;
end
% Step 10: Plot Reflectance and Transmittance
[FIN] = PlotRef(RTE,RTM,EnergyMin,EnergyMax,EnergyDel,ThetaI,C,CG);
[RPB] = PlotTra(TTE,TTM,EnergyMin,EnergyMax,EnergyDel,ThetaI,C,CG);
```

III. MATLAB .M FUNCTION FILES

All the Matlab .m Function files are next listed in alphabetical order.

Angle.m

```
% FUNCTION: Angle
function [Theta] = Angle(ThetaI,IndexP,Index)
Theta = asind((IndexP/Index)*sind(ThetaI));
end
```

Color.m

```
% FUNCTION: Color
function [v] = Color(n,CG)
a = real(n); fff = 1*10-4;
if CG == 1
if a >= -10.0, v = [1 0 0]; end
if a >= -0.10, v = [1 1 1]; end
if a >= fff, v = [1 0 1]; end
if a >= +0.10, v = [0 0 1]; end
if a >= +1.00, v = [0 1 0]; end
if a >= 10.00, v = [1 1 0]; end
if a >= 40.00, v = [0 1 1]; end
if a >= 70.00, v = [0 0 0]; end
else
if a >= -10.0, v = [1 1 1]*0.20; end
if a >= -0.10, v = [1 1 1]*0.30; end
if a >= +0.00, v = [1 1 1]*0.80; end
if a >= +0.10, v = [1 1 1]*0.90; end
if a >= +1.00, v = [1 1 1]*0.95; end
if a >= 10.00, v = [1 1 1]*1.00; end
if a >= 40.00, v = [1 1 1]*1.00; end
if a >= 70.00, v = [1 1 1]*1.00; end
end;
end
```

```

% FUNCTION: DrawMQW
function [L] = DrawMQW(NP,NQ,NF,TP,TQ,TF,DS,CG)
Scale = 70;
figure(1); clf
if CG == 1
BC = [1.0 0.9 0.7]; else
BC = [1 1 1]; end
set(1,'Color',BC)
HA = axes('position',[0.05 0.10 0.35 0.80]);
H = sum(TF) + 100;
HP = plot([0 0 1 1],[0 H H 0],'-k');
set(HP,'Color',BC)
hold on
MI = 0; MA = Scale;
HF = fill([0.3 0.3 0.7 0.7],[MI MA MA MI],Color(NP,CG));
HT = text(0.85,(MI+MA)/2,[sprintf('%4.3f',NP)]);
set(HT,'FontSize',[15],'FontWeight','Bold')
if NP == 0
HT = text(0.1,(MI+MA)/2,'Vacuum'); else
HT = text(0.1,(MI+MA)/2,'Barrier'); end
set(HT,'FontSize',[15],'FontWeight','Bold')
HT = text(0.42,(MI+MA)/2,'Entrance');
set(HT,'FontSize',[15],'FontWeight','Bold')
wsiz = size(TF,2);
MI = MA;
for ws = 1:wsiz
MA = MI + Scale*TF(ws);
HF = fill([0.3 0.3 0.7 0.7],[MI MA MA MI],Color(NF(ws),CG));
HT = text(0.75,(MI+MA)/2,[sprintf('%4.3f',real(NF(ws)))]);
set(HT,'FontSize',[15],'FontWeight','Bold')
if imag(NF(ws)) > 0
HT = text(0.83,(MI+MA)/2,['+_ ' sprintf('%4.3f',imag(NF(ws))) 'i']);
set(HT,'FontSize',[15],'FontWeight','Bold')
end
HT = text(0.2,(MI+MA)/2,[sprintf('%4.2f',TF(ws))]);
set(HT,'FontSize',[15],'FontWeight','Bold')
MI = MA;
end
MA = MI + Scale;
HF = fill([0.3 0.3 0.7 0.7],[MI MA MA MI],Color(NQ,CG));
HT = text(0.85,(MI+MA)/2,[sprintf('%4.3f',NQ)]);
set(HT,'FontSize',[15],'FontWeight','Bold')
if NQ == 0
HT = text(0.1,(MI+MA)/2,'Vacuum'); else
HT = text(0.1,(MI+MA)/2,'Barrier'); end
set(HT,'FontSize',[15],'FontWeight','Bold')
HT = text(0.47,(MI+MA)/2,'Exit');
set(HT,'FontSize',[15],'FontWeight','Bold')
set(HA,'Color',BC,'XColor',BC,'YColor',BC)
HT = title(DS);
set(HT,'FontSize',[15],'FontWeight','Bold')
HX = xlabel('Thickness (nm) ..... P.E. (eV)');
set(HX,'FontSize',[15],'FontWeight','Bold','Color',[0 0 0])
L = 1;
end

```

MatrixA.m

```
% FUNCTION: MatrixA
function [A] = MatrixA(ax,ay,az)
A = zeros(6,6);
A(2,6) = -ax; A(3,5) = +ax; A(5,3) = -ax; A(6,2) = +ax;
A(1,6) = +ay; A(3,4) = -ay; A(4,3) = +ay; A(6,1) = -ay;
A(1,5) = -az; A(2,4) = +az; A(4,2) = -az; A(5,1) = +az;
end
```

MatrixC.m

```
% FUNCTION: MatrixC
function [C] = MatrixC(ep,mu)
C = eye(6,6);
C(3,3) = ep; C(6,6) = mu;
end
```

MatrixM.m

```
% FUNCTION: MatrixM
function [M] = MatrixM(NR,NL,C)
M11 = C; M12 = C*NL;
M21 = C*NR; M22 = C;
M = [M11 M12; M21 M22];
end
```

MatrixMRMT.m

```
% FUNCTION: MatrixMRMT
function [MR,MT] = MatrixMRMT(Q)
Q11 = Q(1:6,1:6); Q12 = Q(1:6,7:12);
Q21 = Q(7:12,1:6); Q22 = Q(7:12,7:12);
MR = Q21*inv(Q11); MT = inv(Q11);
end
```

MatrixN.m

```
% FUNCTION: MatrixN
function [N] = MatrixN(A,W)
N = inv(W)*A;
end
```

MatrixP.m

```
% FUNCTION: MatrixP
function [P] = MatrixP(w,n,theta,hc)
phi = 2*pi*n*(w/hc)*cosd(theta);
P = zeros(12,12);
P(1:6,1:6) = eye(6,6)*exp(+i*phi);
P(7:12,7:12) = eye(6,6)*exp(-i*phi);
end
```

MatrixW.m

```
% FUNCTION: MatrixW
function [W] = MatrixW(ep,mu,n)
W = zeros(6,6);
W(1,1) = -ep/n; W(2,2) = -ep/n; W(3,3) = -ep/n;
W(4,4) = +mu/n; W(5,5) = +mu/n; W(6,6) = +mu/n;
end
```

```

% FUNCTION: PlotRef
function [FIN] = PlotRef(RTE,RTM,LMIN,LMAX,LDEL,THE,C,CG)
x = LMIN:LDEL:LMAX;
HA = axes('position',[0.50 0.50 0.45 0.30]);
if CG == 1
HH = plot(x,100*real(RTE),'-r',x,100*real(RTM),'-b');
else
HH = plot(x,100*real(RTE),'ok',x,100*real(RTM),'xk');
end
set(HH,'LineWidth',[5]); set(HH,'MarkerSize',[1])
Hx = xlabel('K.E. = E-Eo (eV)');
set(Hx,'FontSize',[15],'FontWeight','Bold')
Hy = ylabel('Reflectance (%)');
set(Hy,'FontSize',[15],'FontWeight','Bold')
axis([min(x) max(x) -5 105])
LINC = (LMAX-LMIN)/10;
set(HA,'xtick',[LMIN:LINC:LMAX])
set(HA,'ytick',[0 20 40 60 80 100])
set(HA,'FontSize',[15],'FontWeight','Bold')
set(HA,'LineWidth',[2])
if CG == 1; set(HA,'Color',[0 1 1]); else
set(HA,'Color',[1 1 1]*0.95); end
HT = text(min(x),110,'Spin States:');
set(HT,'FontSize',[15],'FontWeight','Bold')
if CG == 1
HT = text(min(x),110,'.....U');
set(HT,'FontSize',[15],'FontWeight','Bold','Color',[1 0 0])
HT = text(min(x),110,'.....L');
set(HT,'FontSize',[15],'FontWeight','Bold','Color',[0 0 1])
else
HT = text(min(x),110,'.....Uo');
set(HT,'FontSize',[15],'FontWeight','Bold','Color',[0 0 0])
HT = text(min(x),110,'.....Lx');
set(HT,'FontSize',[15],'FontWeight','Bold','Color',[0 0 0])
end
HT = text(min(x),130.0,['Incid = ' sprintf('%4.2f',THE) ' Deg']);
set(HT,'FontSize',[15],'FontWeight','Bold')
HT = text(min(x),150.0,'Richard P. Bocker, Ph.D. ');
set(HT,'FontSize',[15],'FontWeight','Bold')
HT = text(min(x),140.0,'Carlsbad, California, USA');
set(HT,'FontSize',[15],'FontWeight','Bold')
HT = text(min(x),160.0,'Multiple Quantum Well-Barrier Analysis');
set(HT,'FontSize',[15],'FontWeight','Bold'); clc
grid on
FIN = 'Finished';
end

```

PlotTra.m

```
% FUNCTION: PlotTra
function [RPB] = PlotTra(TTE,TTM,LMIN,LMAX,LDEL,THE,C,CG)
x = LMIN:LDEL:LMAX;
HA = axes('position',[0.50 0.10 0.45 0.30]);
if CG == 1
HH = plot(x,100*real(TTE),'-r',x,100*real(TTM),'-b');
else
HH = plot(x,100*real(TTE),'ok',x,100*real(TTM),'xk');
end
set(HH,'LineWidth',[5]); set(HH,'MarkerSize',[1])
Hx = xlabel('K.E.  $\omega$ -E-Eo (eV)');
set(Hx,'FontSize',[15],'FontWeight','Bold')
Hy = ylabel('Transmittance (%)');
set(Hy,'FontSize',[15],'FontWeight','Bold')
axis([min(x) max(x) -5 105])
LINC = (LMAX-LMIN)/10;
set(HA,'xtick',[LMIN:LINC:LMAX])
set(HA,'ytick',[0 20 40 60 80 100])
set(HA,'FontSize',[15],'FontWeight','Bold')
set(HA,'LineWidth',[2])
if CG == 1; set(HA,'Color',[0 1 1]); else
set(HA,'Color',[1 1 1]*0.95); end
grid on
RPB = 'Thats all Folks'; clc
end
```

PsiI.m

```
% FUNCTION: PsiI
function [PsiI_TE,PsiI_TM] = PsiI(ThetaI,epP,muP)
R = sqrt(epP/muP); S = sqrt(muP/epP);
Vec_TE = [0 1 0 +R*cosd(ThetaI) 0 -R*sind(ThetaI)].';
Vec_TM = [-S*cosd(ThetaI) 0 +S*sind(ThetaI) 0 1 0].';
PsiI_TE = Vec_TE/sqrt(Vec_TE'*Vec_TE);
PsiI_TM = Vec_TM/sqrt(Vec_TM'*Vec_TM);
end
```

IV. MATLAB .M SCRIPT FILES

Matlab .m Script files are next listed in alphabetical order.

Convert.m

```
% SCRIPT: Convert
% Conversion of EM Quantities to QM Quantities
% Introduce Relativistic Lorentz Factor
UP = PotentP; UQ = PotentQ; UF = PotentF;
gP = (E - UP)/Eo; gQ = (E - UQ)/Eo; gF = (E - UF)/Eo;
epP = (gP + 1)*Eo; muP = (gP - 1)*Eo;
epQ = (gQ + 1)*Eo; muQ = (gQ - 1)*Eo;
epF = (gF + 1)*Eo; muF = (gF - 1)*Eo;
IndexP = sqrt(epP.*muP);
IndexQ = sqrt(epQ.*muQ);
IndexF = sqrt(epF.*muF);
pc = sqrt(gF + 1).*sqrt(gF - 1)*Eo;
```

MatrixQ.m

```
% SCRIPT: MatrixQ
Q = inv(MIR);
for n = 1:N
Q = Q*Mn(:, :, n)*inv(Pn(:, :, n))*inv(Mn(:, :, n));
end
Q = Q*MIT;
```

Phases.m

```
% SCRIPT: Phases
for n = 1:N
[Pn(:, :, n)] = MatrixP(ThickF(n), pc(n), ThetaF(n), hc);
end
```

Prelim.m

```
% SCRIPT: Prelim
disp(' _Matlab:_Multiple_Quantum_Well-and-Barrier_Analysis_Program')
disp(' _Author:_Richard_P._Bocker,_Ph.D. ')
disp(' _ '); disp(' _Begin_Calculations '); disp(' _ ')
c = 3.00*10^8; % Speed of Light in Vacuum (m/s)
h = 4.14*10^-15; % Planck Constant (eV*s)
Me = 9.11*10^-31; % Electron Rest Mass (kg)
Eo = 5.12*10^5; % Electron Rest Mass Energy (eV)
hc = 1.241*10^3; % (eV*nm)
Mecc = 0.511*10^6; % (eV)
ThetaI = 0.00; % (degrees)
CG = input(' _Type_1_for_Color_or_2_for_Gray_Plots:_ ');
```


Probability.m

```
% SCRIPT: Probability
AA = PsiR_TE; BB = PsiI_TE; CC = PsiR_TM; DD = PsiI_TM;
EE = PsiT_TE; FF = PsiT_TM;
NUM = sqrt(AA(1:3)'*AA(1:3))*sqrt(AA(4:6)'*AA(4:6));
DEN = sqrt(BB(1:3)'*BB(1:3))*sqrt(BB(4:6)'*BB(4:6));
RTE(L) = (NUM/DEN);
NUM = sqrt(CC(1:3)'*CC(1:3))*sqrt(CC(4:6)'*CC(4:6));
DEN = sqrt(DD(1:3)'*DD(1:3))*sqrt(DD(4:6)'*DD(4:6));
RTM(L) = (NUM/DEN);
NUM = sqrt(EE(1:3)'*EE(1:3))*sqrt(EE(4:6)'*EE(4:6));
DEN = sqrt(BB(1:3)'*BB(1:3))*sqrt(BB(4:6)'*BB(4:6));
TTE(L) = (NUM/DEN)*Ratio;
NUM = sqrt(FF(1:3)'*FF(1:3))*sqrt(FF(4:6)'*FF(4:6));
DEN = sqrt(DD(1:3)'*DD(1:3))*sqrt(DD(4:6)'*DD(4:6));
TTM(L) = (NUM/DEN)*Ratio;
clear AA BB CC DD EE FF
L = L + 1;
```

RegionF.m

```
% SCRIPT: RegionF
for n = 1:N
[ThetaF(n)] = Angle(ThetaI, IndexP, IndexF(n));
[CF] = MatrixC(1,1);
[WF] = MatrixW(epF(n), muF(n), IndexF(n));
[AFR] = MatrixA(cosd(90-ThetaF(n)), 0, cosd(ThetaF(n)));
[AFL] = MatrixA(cosd(90-ThetaF(n)), 0, cosd(180-ThetaF(n)));
[NFR] = MatrixN(AFR, WF);
[NFL] = MatrixN(AFL, WF);
[Mn(:, :, n)] = MatrixM(NFR, NFL, CF);
end
```

RegionP.m

```
% SCRIPT: RegionP
[CP] = MatrixC(1,1);
[WP] = MatrixW(epP, muP, IndexP);
[APR] = MatrixA(cosd(90-ThetaI), 0, cosd(ThetaI));
[APL] = MatrixA(cosd(90-ThetaI), 0, cosd(180-ThetaI));
[NPR] = MatrixN(APR, WP);
[NPL] = MatrixN(APL, WP);
[MIR] = MatrixM(NPR, NPL, CP);
```

RegionQ.m

```
% SCRIPT: RegionQ
[ThetaT] = Angle(ThetaI, IndexP, IndexQ);
[CQ] = MatrixC(1,1);
[WQ] = MatrixW(epQ, muQ, IndexQ);
[AQR] = MatrixA(cosd(90-ThetaT), 0, cosd(ThetaT));
[AQL] = MatrixA(cosd(90-ThetaT), 0, cosd(180-ThetaT));
[NQR] = MatrixN(AQR, WQ);
[NQL] = MatrixN(AQL, WQ);
[MIT] = MatrixM(NQR, NQL, CQ);
Ratio = cosd(ThetaT)/cosd(ThetaI);
```

```
% SCRIPT: Structure
disp('Following Examples Illustrate Software Capability:')
disp('Code_01: MQW01: Layers_01: Finite Qunatum Barrier')
disp('Code_02: MQW02: Layers_01: Finite Quantum Well')
disp('Code_03: MQW03: Layers_03: Quantum Barrier Tunneling')
disp('Code_04: MQW04: Layers_03: Finite Quantum Well')
disp('Code_05: MQW05: Layers_07: Well-and-Barrier Structure')
disp('Code_06: MQW06: Layers_11: Scattering-Periodic Potential')
C = input('Type in Two-Digit SUB-Structure Code Number: ');
if C == 01; MQW01; end; if C == 02, MQW02; end
if C == 03, MQW03; end; if C == 04, MQW04; end
if C == 05, MQW05; end; if C == 06, MQW06; end
```

```
% SCRIPT: Wavefunction
PsiR_TE = MR*PsiI_TE;
PsiR_TM = MR*PsiI_TM;
PsiT_TE = MI*PsiI_TE;
PsiT_TM = MI*PsiI_TM;
```

V. MATLAB .M SCRIPT FILES - EXAMPLES

In addition, there are six Matlab .m Script files depicting examples of different multilayer quantum well-and-barrier structures. One can easily add more to this list by examining the content of these files as well as the Structure.m script file.

```
% SCRIPT: MQW01
DS = 'MQW01: Finite Quantum Barrier (1 Layer)';
N = 1; % Number of Thin-Film Layers
EnergyMin = 0.00; % Minimum Particle Energy (eV)
EnergyMax = 80.00; % Maximum Particle Energy (eV)
EnergyDel = 0.10; % Energy Increment (eV)
ThickP = 0.20; % Region P Gap Width (nm)
PotentP = 0.00; % Region P Potential Energy (eV)
ThickQ = 0.20; % Region Q Gap Width (nm)
PotentQ = 0.00; % Region Q Potential Energy (eV)
ThickF = [0.20]; % Thin-Film Thickness (nm)
PotentF = [40.0]; % Thin-Film Potential Energy (eV)
```

```
% SCRIPT: MQW02
DS = 'MQW02: Finite Quantum Well (1 Layer)';
N = 1; % Number of Thin-Film Layers
EnergyMin = 0.00; % Minimum Particle Energy (eV)
EnergyMax = 8.00; % Maximum Particle Energy (eV)
EnergyDel = 0.01; % Energy Increment (eV)
ThickP = 1.00; % Region P Gap Width (nm)
PotentP = 0.00; % Region P Potential Energy (eV)
ThickQ = 1.00; % Region Q Gap Width (nm)
PotentQ = 0.00; % Region Q Potential Energy (eV)
ThickF = [1.50]; % Thin-Film Thickness (nm)
PotentF = [-3.00]; % Thin-Film Potential Energy (eV)
```

MQW03.m

```

% SCRIPT: MQW03
DS = 'MQW03: QuantumBarrierTunneling_(3_Layers)';
TFT = [0.25 0.50 0.25];
TFE = [10.0 0.00 10.0];
N = 3; % Number of Thin-Film Layers
EnergyMin = 0.00; % Minimum Particle Energy (eV)
EnergyMax = 16.00; % Maximum Particle Energy (eV)
EnergyDel = 0.004; % Energy Increment (eV)
ThickP = 0.50; % Region P Gap Width (nm)
PotentP = 0.00; % Region P Potential Energy (eV)
ThickQ = 0.50; % Region Q Gap Width (nm)
PotentQ = 0.00; % Region Q Potential Energy (eV)
ThickF = TFT; % Thin-Film Thicknesses (nm)
PotentF = TFE; % Thin-Film Potential Energies (eV)
clear TFT TFE

```

MQW04.m

```

% SCRIPT: MQW04
DS = 'MQW04: QuantumWellEnergyLevels_(3_Layers)';
vvv = 1.00;
aaa = sqrt((49*hc*hc)/(128*Mecc*vvv));
TFT = [1 2 1];
TFE = [1 0 1];
N = 3; % Number of Thin-Film Layers
EnergyMin = 0.00; % Minimum Particle Energy (eV)
EnergyMax = 2.00; % Maximum Particle Energy (eV)
EnergyDel = 0.001; % Energy Increment (eV)
ThickP = 5.00; % Region P Gap Width (nm)
PotentP = 0.00; % Region P Potential Energy (eV)
ThickQ = 5.00; % Region Q Gap Width (nm)
PotentQ = 0.00; % Region Q Potential Energy (eV)
ThickF = TFT*aaa; % Thin-Film Thicknesses (nm)
PotentF = TFE*vvv; % Thin-Film Potential Energies (eV)
clear vvv aaa TFT TFE

```

MQW05.m

```

% SCRIPT: MQW05
DS = 'MQW05: Well-and-BarrierStructure_(7_Layers)';
TFT = [2.5 1 1.5 1 1.5 1 2.5]*0.3;
TFE = [.5 0 1 0 1 0 .5]*2.0;;
N = 7; % Number of Thin-Film Layers
EnergyMin = 0.00; % Minimum Particle Energy (eV)
EnergyMax = 3.00; % Maximum Particle Energy (eV)
EnergyDel = 0.003; % Energy Increment (eV)
ThickP = 1.00; % Region P Gap Width (nm)
PotentP = 0.00; % Region P Potential Energy (eV)
ThickQ = 1.00; % Region Q Gap Width (nm)
PotentQ = 0.00; % Region Q Potential Energy (eV)
ThickF = TFT; % Thin-Film Thicknesses (nm)
PotentF = TFE; % Thin-Film Potential Energies (eV)
clear TFT TFE

```

```

% SCRIPT: MQW06
DS = 'MQW06: Scattering-Periodic-Potential_(11_Layers)';
TFT = [1 1 1 1 1 1 1 1 1 1 1]*0.3;
TFE = [1 0 1 0 1 0 1 0 1 0 1]*2.0;
N = 11; % Number of Thin-Film Layers
EnergyMin = 0.00; % Minimum Particle Energy (eV)
EnergyMax = 4.00; % Maximum Particle Energy (eV)
EnergyDel = 0.004; % Energy Increment (eV)
ThickP = 1.00; % Region P Gap Width (nm)
PotentP = 0.00; % Region P Potential Energy (eV)
ThickQ = 1.00; % Region Q Gap Width (nm)
PotentQ = 0.00; % Region Q Potential Energy (eV)
ThickF = TFT; % Thin-Film Thicknesses (nm)
PotentF = TFE; % Thin-Film Potential Energies (eV)
clear TFT TFE

```