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clear
close all
clc
figure('Units','normalized','OuterPosition',[0 0 1
1],'NumberTitle','off')

%defining constants
hbar=1.0546e-34;
m0=9.1e-31;
e=1.6e-19;

%forming a task
L=1e-8; %width of structure
Np=1000; %amount of steps
x=linspace(-L/2,L/2, Np); %creating a 'x-axis'
dx=x(2)-x(1); %definig a primive step
koef=-hbar^2/(2*m0*12*(dx^2)); %definig a coefficient for analytical
    solving

%defining potential feild
U=zeros(1,Np);
Upetr=[zeros(1,Np/2), ones(1,Np/2)*0.01*e];
%these fields are considered to be default
%Upetr=0.01*e*(1+sin(pi*10*x/L));

%numerical solution for hamiltonian
E=eye(Np)*(-30);
E=E+diag(ones(1,Np-1)*16,-1);
E=E+diag(ones(1,Np-1)*16,1);
E=E+diag(ones(1,Np-2)*(-1),-2);
E=E+diag(ones(1,Np-2)*(-1),2);

%Hamiltonian
H=E*koef+diag(U);
Hpetr=E*koef+diag(U+Upetr);

%finding eigenvalues and eigenvectors
[P,En]=eig(H);
[Ppetr,Enpetr]=eig(Hpetr);
En=diag(En);
Enpetr=diag(Enpetr);

%Finding an amendment given by perturbation
n=P(:,1);
dE1=n'*diag(Upetr)*n/e; %first attempt to energy
dn=0; dE2=0;
for i=2:10 %first attempt to function and second for
    energy
        k=P(:,i);
        dn=dn+(k'*diag(Upetr)*n)./(En(1)-En(i))*k;
        dE2=dE2+(k'*diag(Upetr)*n)./(En(1)-En(i))*(n'*diag(Upetr)*k);
end

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dE2=dE2/e;%J->eV

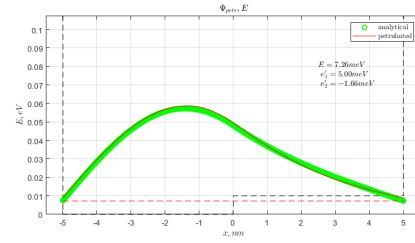
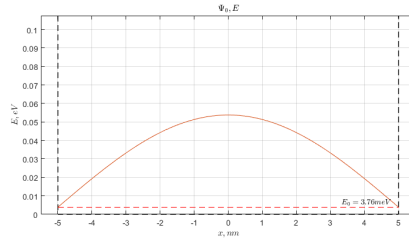
%visualization
%non-petrubated state
subplot(2,2,1)
hold off
plot([-L/2-dx -L/2 x L/2 L/2+dx]*1e9, [0.25 0.25 U/e 0.25 0.25], '--k', 'LineWidth', 1)
hold on;
[~,zx]=max(abs(P(:,1)));
amp=P(zx,1);%defining amplitude for scaling a wave-function
for i=1:1
    plot(x*1e9, En(i)/e+0.05*P(:,i)/amp);
    plot(x*1e9, En(i)*ones(1,Np)/e,'--r');
end
E1=En(1)/e;%J->eV
xlabel('$x, nm$', 'Interpreter', 'latex');
ylabel('$E, eV$', 'Interpreter', 'latex');
title('$\Psi_0, E$', 'Interpreter', 'latex');
text((sum(xlim) + diff(xlim))/2-0.2*(diff(xlim)-sum(xlim))/2, En(1)/e,...
    sprintf('$E_0 = %2.2f meV$', E1*1000), 'Interpreter', 'latex', ...
    'HorizontalAlignment', 'right', 'VerticalAlignment', 'bottom')
grid on;
ylim([0 2*(E1+0.05)])
xlim([-L/2*1.1 L/2*1.1]*1e9)

subplot(2,2,2)
hold off
plot([-L/2-dx -L/2 x L/2 L/2+dx]*1e9, [0.15 0.15 Upetr/e 0.15 0.15], '--k', 'HandleVisibility','off')
hold on;
%pseudoanalytical solution
[~,zx]=max(abs(Ppetr(:,1)));%defining amplitude for scaling a wave-function
amp=Ppetr(zx,1);
plot(x*1e9, Enpetr(1)/e+0.05*Ppetr(:,1)/amp(1), 'go', 'LineWidth', 1.5, 'HandleVisibility', 'on');
P=n+dn;
%petrubation theory solution
amp=(max(abs(P)));
plot(x*1e9, (En(1)/e+dE1)+0.05*(abs(P))/amp, 'r');
legend('analytical', 'petrubated', 'Interpreter', 'latex');
plot(x*1e9, Enpetr(1)*ones(1,Np)/e, '--r', 'HandleVisibility', 'off');
E2=Enpetr(1)/e;
xlabel('$x, nm$', 'Interpreter', 'latex');
ylabel('$E, eV$', 'Interpreter', 'latex');
title('$\Psi_{\{petr\}}, E$', 'Interpreter', 'latex');
grid on;
ylim([0 2*(E1+0.05)])
text((sum(xlim) + diff(xlim))/2-0.5*(diff(xlim)-sum(xlim))/2, 0.7*sum(ylim), ...
    sprintf('$E = %2.2f meV$ \n $E_1 = %2.2f meV$ \n $E_2 = %2.2f meV$', [E2,dE1,dE2]*1000), 'Interpreter', 'latex')

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xlim([-L/2*1.1 L/2*1.1]*1e9)
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%verification of WF by comparison energies
Err = uicontrol('style','text');
txtterr=sprintf("Estimated Energy in perturbation: E= Eo +e1+e2=
%2.2fmeV\nCalculation error is %2.2f%%",...
    [(E1+dE1+dE2)*1e3,abs((( -E2+E1+dE1+dE2)/E2)*100)]);
set(Err,'String',txtterr,'FontSize',14,'FontWeight','bold');
Err.Units='normalized';
Err.Position=[0.15 0.2 0.3 0.1];
```



Estimated Energy in perturbation: E= Eo +e1+e2=7.09meV
Calculation error is 2.33%

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