```
clear
close all
clc
datestr(now)
figure('Units', 'normalized', 'OuterPosition', [0 0 1 1]);

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

%forming a task
L=1e-8;
Np=1000;
x=linspace(-L/2,L/2, Np);
dx=x(2)-x(1);
koef=-hbar^2/(2*m0*12*(dx^2));

%defining potential feild
type=2;
switch type
    case 2
        U=abs(x/(L/2)*e/2);
    case 1
        U=e/2-abs(x/(L/2)*e/2);
    case 3
        U=e/2*(1+sin(pi*10*x/L));
    case 4
        U=e/2*(exp(-x.^2/(L/10)^2));
    case 5
        U=heaviside(x)*e/100;
end

%numerical solution for hamiltonian
    %defining secind devirative
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);

%finding eigenvalues and eigenvectors
[P,Ei]=eig(H);
Ei=diag(Ei);

%choosing 10 solutions of particle in a box as a basis
Count=10;
m=1:Count;
phi=sqrt(2/L)*sin(pi/2*m+pi*x'*m/L);
```

```
phi=phi./sqrt(diag(phi'*phi)');

%solving variation
%declaring matrixes
Hij=phi'*H*phi;
Sij=phi'*phi;
%solving for minimal E
syms E
E=double(solve(det(Hij-E*Sij)==0));
Em=E(1);
%determenating constants
c=null((Hij-Em*Sij));
Psi=phi*c;

%plotting analytical main state
subplot(2,6,1:3)
hold off
plot(x*1e9, U/e, '--k', 'LineWidth', 1)
hold on;
Amp=P(islocalmax(abs(P(:,1))),1);
for i=1:1
    plot(x*1e9, Ei(i)/e+0.1*P(:,i)/Amp,'-');
    plot(x*1e9, Ei(i)*ones(1,Np)/e,'--r');
    text(-4.5,Ei(i)/e,sprintf('$E_%i = %2.2f meV$',[i Ei(i)/
e*1000]),...
        'Interpreter','latex','FontSize',14,...
        'HorizontalAlignment','left','VerticalAlignment','bottom')
end
xlabel('$x,nm$', 'Interpreter', 'latex');
ylabel('$E,eV$', 'Interpreter', 'latex');
title('$Numreical$ $\Psi,E$', 'Interpreter', 'latex');
E1=Ei(1);
grid on;

%plotting methods main state
subplot(2,6,4:6)
hold off
plot(x*1e9, U/e, '--k', 'LineWidth', 1)
hold on
Psi=abs(Psi');
Amp=Psi(islocalmax(abs(Psi)));
plot(x*1e9,Em/e+0.1*Psi/max(Amp))
plot(x*1e9, Em/e*ones(1,Np),'--r');
text(-4.5,Em/e,sprintf('$E_{var} = %2.2f meV$',Em/
e*1000),'Interpreter','latex',...
'FontSize',14,'HorizontalAlignment','left','VerticalAlignment','bottom')
xlabel('$x,nm$', 'Interpreter', 'latex');
ylabel('$E,eV$', 'Interpreter', 'latex');
title('$Variated$ $\Psi,E$', 'Interpreter', 'latex');
grid on;

%plotting basis functions
subplot(2,6,11:12)
bar(c);
```

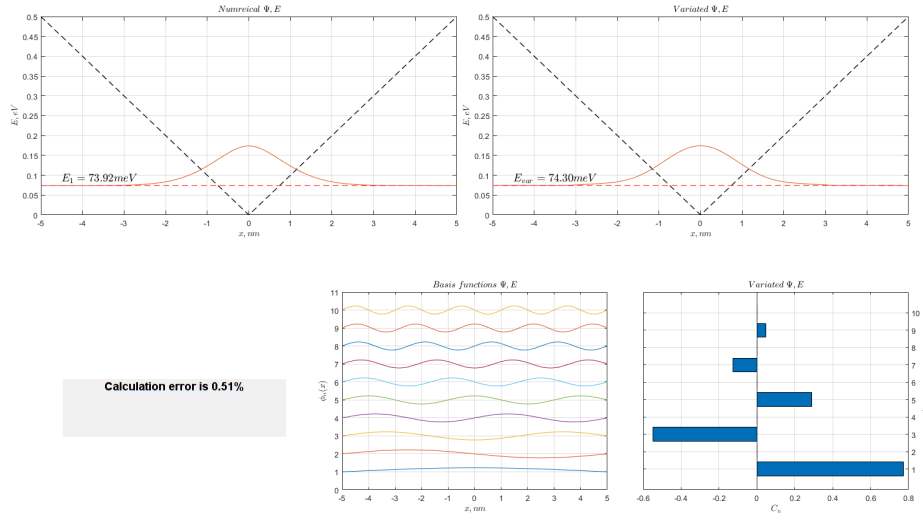
```
xlabel('$n^{th}$ $component$', 'Interpreter', 'latex');
ylabel('$C_n$', 'Interpreter', 'latex');
title('$Variated$ $\Psi,E$', 'Interpreter', 'latex');
grid on;
camroll(90)
set(gca,'YDir','reverse')

%plotting basis functions' coeffisients
subplot(2,6,9:10)
plot(ones(1,Count).*x'*1e9,5*phi+m)
xlabel('$x,nm$', 'Interpreter', 'latex');
ylabel('$\phi_n(x)$', 'Interpreter', 'latex');
title('$Basis$ $functions$ $\Psi,E$', 'Interpreter', 'latex');
grid on;
ylim([0 Count+1])

%verification of WF by comparison energies
Err = uicontrol('style','text');
txterr=sprintf('Calculation error is %2.2f%%',((Em-E1)/E1*100));
set(Err,'String',txterr,'FontSize',14,'FontWeight','bold');
Err.Units='normalized';
Err.Position=[0.15 0.20 0.2 0.1];
clear
```

```
ans =

    '29-Nov-2021 00:10:46'
```



Published with MATLAB® R2020b