Assignment 03

Many Body Wave Function of Two Electrons in Potential Well

Submitted by

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1. **Theory**
   a. Non interacting particles

When we put two identical particles in the box, if they were classical particles, we can tell the particles apart. In quantum mechanics, this is no longer possible because all we can predict is the probability that one of the particles is in a region dx_1 about the point x_1 and the other is in a region dx_2 about the point x_1, but we cannot tell which particle is where. This fact affect both the allowed energies and the wave functions.

The classical energy inside the box is, in this case

$$\frac{p_1^2}{2m} + \frac{p_1^2}{2m}$$

where p_1 is the momentum of particle 1, and p_2 is the momentum of particle 2. Because the energy is a sum of independent energies for particles 1 and 2, the energies can also be separated

$$E = \varepsilon_1 + \varepsilon_2$$

The wave function will depend on the positions x_1 and x_2, $\psi(x_1,x_2)$, and therefore, we have four boundary conditions $\psi(x_1,0) = 0$, $\psi(0,x_2) = 0$, $\psi(x_1,L) = 0$, and $\psi(L,x_2) = 0$. These give rise to the allowed values of ε_1 and ε_2 of,

$$\varepsilon_1 = \frac{\hbar^2\pi^2}{2mL^2} n_1^2$$

$$\varepsilon_2 = \frac{\hbar^2\pi^2}{2mL^2} n_2^2$$

so that the allowed values of the total energy are

$$E_{n1,n2} = \frac{\hbar^2\pi^2}{2mL^2} (n_1^2 + n_2^2)$$

We cannot express the wave functions to be a simple product

$$\Psi_{n1n2}(x_1, x_2) = \psi_{n1}(x_1)\psi_{n2}(x_2)$$

because x_1 and x_2 are not independent of one another. the simple product form says that there are points at which $\Psi_{n1n2}(x, x) \neq 0$, implying that there is a nonzero probability of finding the two particles at exactly the same point in space, i.e. sitting right on top of each other. Also the simple product wave function above specifies a definite assignment of n_1 to particle 1 and n_2 to particle 2. But if the particle are truly identical, this should not be possible.

Generally two possible product forms is considered, i.e. $\psi_{n1}(x_1)\psi_{n2}(x_2)$ and $\psi_{n2}(x_1)\psi_{n1}(x_2)$ which are put together to form $\Psi_{n1n2}(x_1, x_2)$. It can be done in two ways:

$$\Psi_{n1n2}(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n1}(x_1)\psi_{n2}(x_2) \pm \psi_{n2}(x_1)\psi_{n1}(x_2)]$$

If we take the first one:

$$\Psi_{n1n2}(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n1}(x_1)\psi_{n2}(x_2) + \psi_{n2}(x_1)\psi_{n1}(x_2)]$$

it will still be possible for the two particle to sit at the same point in space. In fact, there are certain exotic particles in quantum mechanics that can do this and called *bosons*. However, for *fermions*, which cannot sit on top of each other, we need to take the second form

$$\Psi_{n1n2}(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n1}(x_1)\psi_{n2}(x_2) - \psi_{n2}(x_1)\psi_{n1}(x_2)]$$

This form implies two things.

$$\Psi_{n1n2}(x, x) = 0$$

which means that for any n_1 and n_2, there is zero probability to find both particles in small regions near the same point. The other thing we see is that

$$\Psi_{nn}(x_1, x_2) = 0$$

which implies that the two particles cannot be in the same energy level which is *Pauli exclusion principle*.

b. Interacting particles

In the above case it is considered that the two particle are not interacting with one another. But for electron, which is a *fermion*, there is a coulomb interaction. To see the effect of this potential we need to include the coulomb interaction term in the Schrodinger equation –

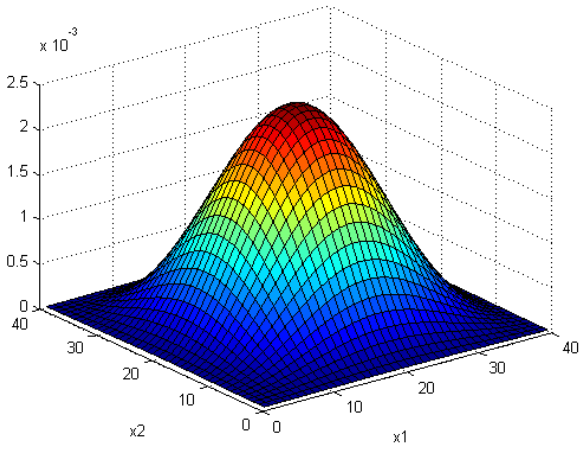
$$-\frac{\hbar^2}{2m}\left(\frac{d}{dx_1} + \frac{d}{dx_2}\right)\Psi(x_1, x_2) + \frac{e}{4\pi\epsilon_0|x_1 - x_2|} = \varepsilon\Psi(x_1, x_2)$$

2. Simulation Result

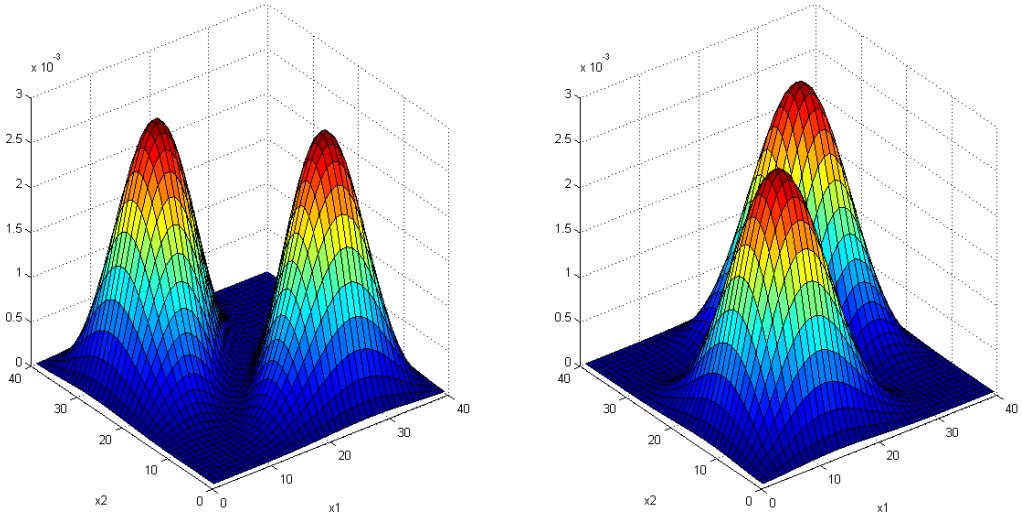
a. Non interacting particles

Well length = 4 nm
Mesh size = 0.1 nm

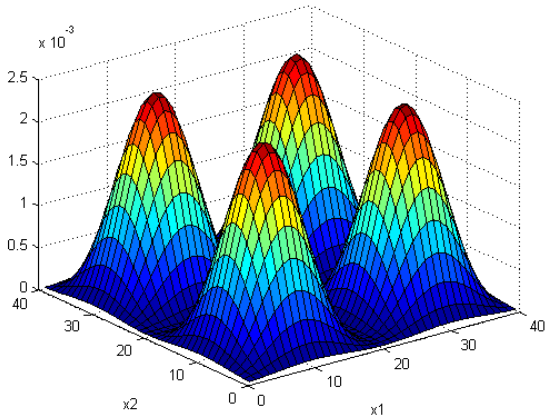
The following graphs are the wave function $\Psi_{n1n2}(x_1, x_2)$ for different n_1 and n_2.



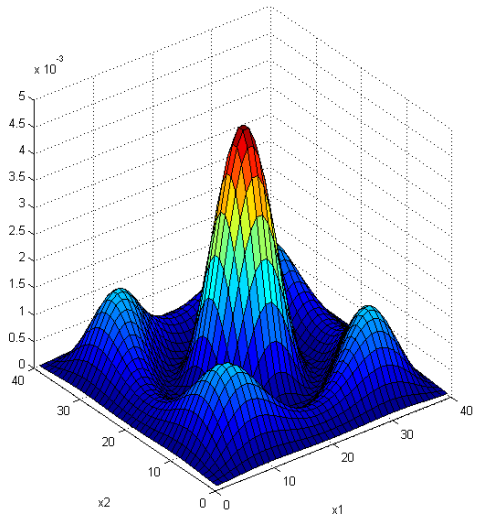
$n_1 = n_2 = 1$; *boson*

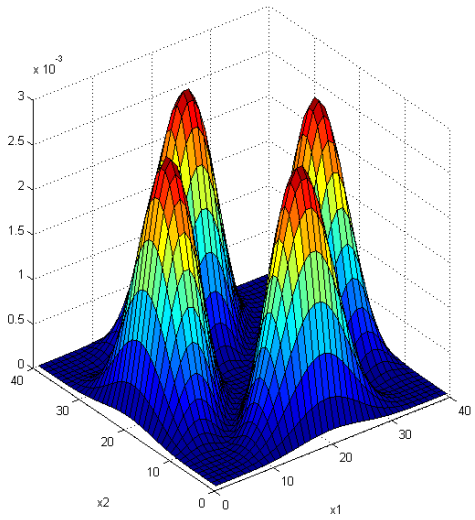


$n_1 = 1$, $n_2 = 2$ or vice versa; (*left*) *fermion* (*right*) *boson*

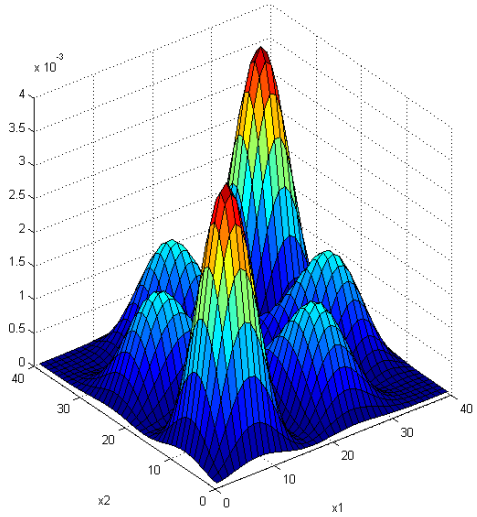


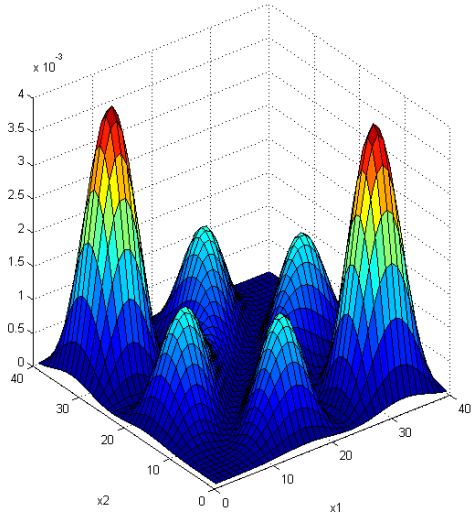
$n_1 = n_2 = 2$; *boson*





$n_1 = 1$, $n_2 = 3$ or vice versa; (*left*) *boson (right) fermion*





$n_1 = 2$, $n_2 = 3$ or vice versa; (*left*) *boson (right) fermion*

We see that *boson* can occupy the same energy state and two *boson* particles can exist at the same point as if they are stacked upon one another. Also, *fermion* does not occupy all the energy state possible, for example, the energy of the ground state for fermion is $5E_0$, and not $2E_0$, where,

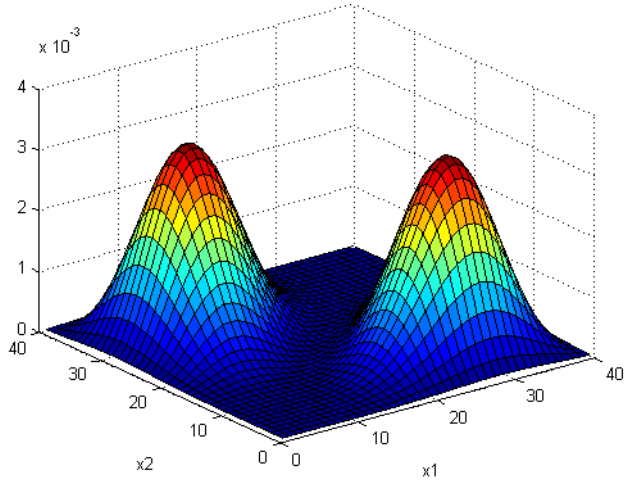
$$E_0 = \frac{\hbar^2 \pi^2}{2mL^2}$$

Below is the theoretical and calculated eigen value –

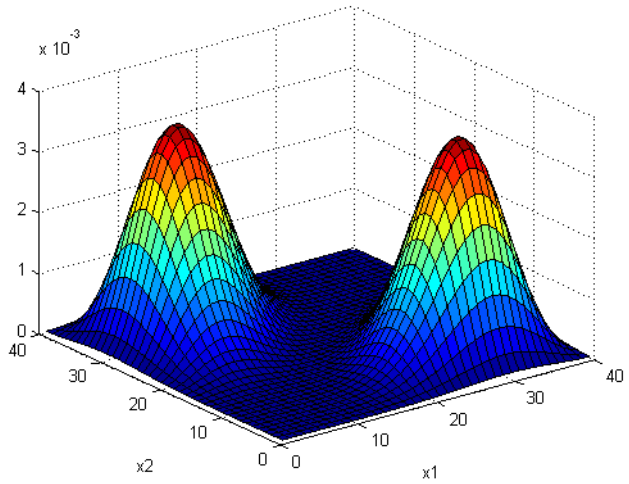
Eigen vector	Calculated value	Theoretical value
Ψ_{11}	-0.0449	-0.0472
$\Psi_{12} = \Psi_{21}$	-0.1121	-0.1179
Ψ_{22}	-0.1792	-0.1887
$\Psi_{13} = \Psi_{31}$	-0.2236	-0.2357
$\Psi_{23} = \Psi_{32}$	-0.2908	-0.3066

b. Interacting particles

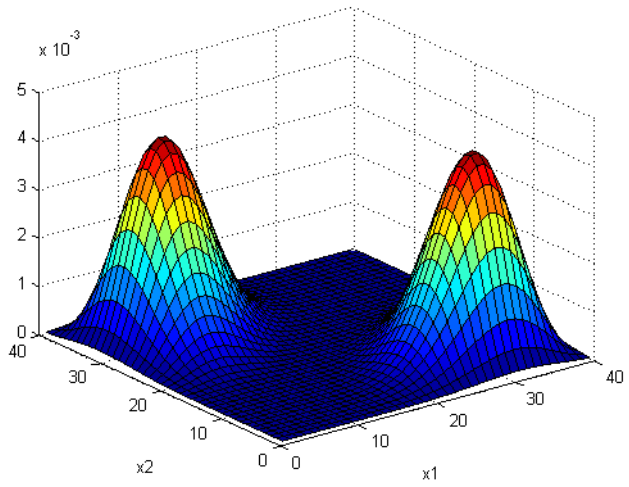
For interacting particles we can see the influence of the size of the well on the many body wave function. Following figures are the ground state eigen state at different well length



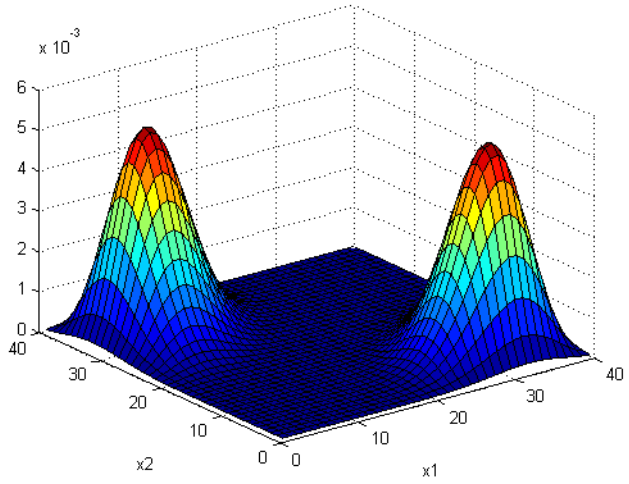
L = 0.25 nm



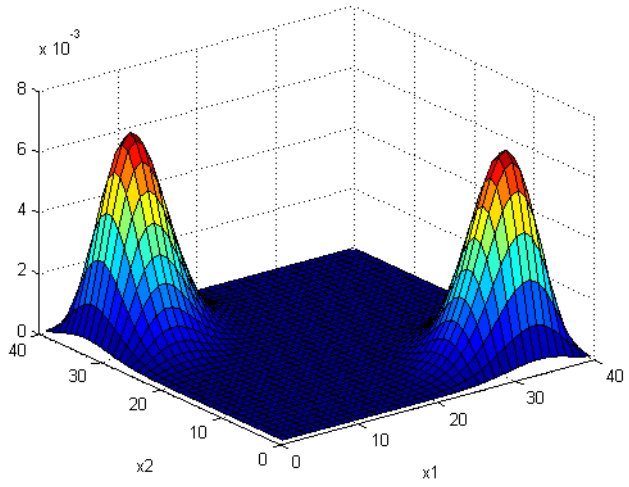
L = 0.50 nm



L = 1.00 nm



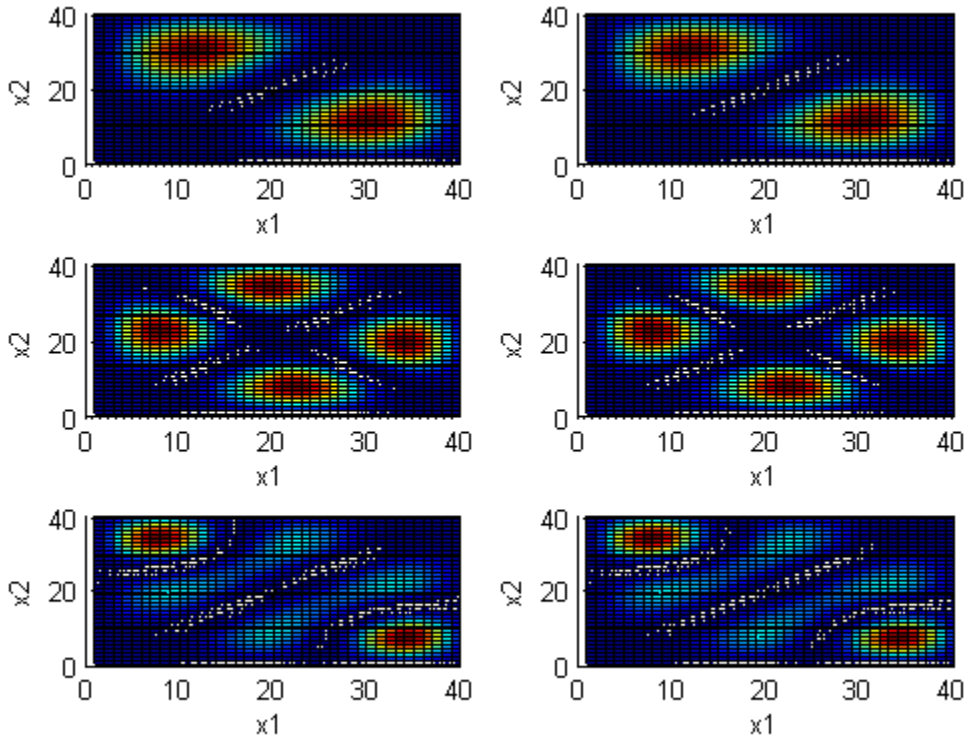
L = 2.00 nm



L = 4.00 nm

It is clear that as length of the well increases the electron are move further apart from each other due to coulomb repulsion force. The probability is maximum when the two particles are further apart.

There are no *bosonic* many body wave function in the solution. For clarification, in the following figure we show the first six eigen state in a contour plot for well length L = 0.25 nm. As we see there is non-zero probability for $\Psi_{n1n2}(x, x)$.



First six eigen state for L = 0.25 nm

Following table shows the eigen values for ground state at different well length

Well length(nm)	Eigen value(eV)
.25	-45.4098
.50	-15.0160
1.00	-5.3748
2.00	-2.0528
4.00	-0.8262

Following table shows the eigen values for first six state at well length 0.25 nm

Eigen state	Eigen value(eV)
$\Psi_{12} = \Psi_{21}$	-45.4098
$\Psi_{13} = \Psi_{31}$	-78.2757
$\Psi_{23} = \Psi_{32}$	-93.7976

3. Code

a. Non interacting particles

```
      close all;
clear all;
clc;

% constants
hcut =  6.63 * (10 ^ -34) / (2 * pi);
m = 9.1 * (10 ^ -31);
e = 1.6 * (10^-19);

% defining the mesh
nm = 10^-9;
dx = 0.1 * nm;                    % mesh size
x1 = -2*nm:dx:2*nm-dx;               % defining the x1 dimension (-2nm - 2nm)
N = length(x1);


k = - hcut^2 / (2 * m * e * dx^2);
%% defining the kinetic energy matrix
%%% used dirichlet boundary condition
B = (diag(ones(1,N)*4)-diag(ones(1,N-1),1)-diag(ones(1,N-1),-1));
I = -eye(N, N);
H = zeros(N^2, N^2);

for i = 2:N-1
    H((i-1)*N + 1:(i)*N, (i-2)*N + 1:(i-1)*N) = I;
    H((i-1)*N + 1:(i)*N, (i-1)*N + 1:(i)*N) = B;
    H((i-1)*N + 1:(i)*N, (i)*N + 1:(i+1)*N) = I;
end
H(1:N,1:N) = B;
H(1:N, N+1:2*N) = I;
H((N-1)*N + 1:N^2,(N-2)*N + 1:(N-1)*N) = I;
H((N-1)*N + 1:N^2,(N-1)*N + 1:N^2) = B;

H = k*H;

%% eigensolver
[WF, En] = eig(H);

%% GRAPHS
psi = reshape(WF(:, N^2), N, N);
psi1 = reshape(WF(:, N^2-1), N, N);
psi2 = reshape(WF(:, N^2-2), N, N);
psi3 = reshape(WF(:, N^2-3), N, N);
psi4 = reshape(WF(:, N^2-4), N, N);
psi5 = reshape(WF(:, N^2-5), N, N);
psi6 = reshape(WF(:, N^2-6), N, N);
psi7 = reshape(WF(:, N^2-7), N, N);

figure(1)
surf(psi.^2)
%view([0 90])
```

```
xlabel('x1')
ylabel('x2')

figure(2)
subplot(121)
surf(psi1.^2)
%view([0 90])
xlabel('x1')
ylabel('x2')

subplot(122)
surf(psi2.^2)
%view([0 90])
xlabel('x1')
ylabel('x2')


figure(4)
surf(psi3.^2)
%view([0 90])
xlabel('x1')
ylabel('x2')

figure(5)
subplot(121)
surf(psi4.^2)
%view([0 90])
xlabel('x1')
ylabel('x2')

subplot(122)
surf(psi5.^2)
%view([0 90])
xlabel('x1')
ylabel('x2')

figure(6)
subplot(121)
surf(psi6.^2)
%view([0 90])
xlabel('x1')
ylabel('x2')

subplot(122)
surf(psi7.^2)
%view([0 90])
xlabel('x1')
ylabel('x2')
%% energy
E = diag(En);
```

b. Interacting particles

```
close all;
clear all;
clc;

% constants
hcut =  6.63 * (10 ^ -34) / (2 * pi);
m = 9.1 * (10 ^ -31);
e = 1.6 * (10^ -19);
e0 = 8.854 * (10 ^ -12);

E = zeros(1, 5);
E25 = zeros(1, 6);
for p = 1:5
% defining the mesh
nm = 10^-9;
d = 2^(p-1);
dx = d*0.00625 * nm;                          % mesh size
x1 = -d*0.125*nm:dx:d*0.125*nm-dx;            % defining the x1 dimension
N = length(x1);


k = - hcut^2 / (2 * m * e * dx^2);
C = - e / (4 * pi * e0);
%% defining the kinetic energy matrix
%%% used dirichlet boundary condition
B = (diag(ones(1,N)*4)-diag(ones(1,N-1),1)-diag(ones(1,N-1),-1));
I = -eye(N, N);
H = zeros(N^2, N^2);

for i = 2:N-1
    H((i-1)*N + 1:(i)*N, (i-2)*N + 1:(i-1)*N) = I;
    H((i-1)*N + 1:(i)*N, (i-1)*N + 1:(i)*N) = B;
    H((i-1)*N + 1:(i)*N, (i)*N + 1:(i+1)*N) = I;
end
H(1:N,1:N) = B;
H(1:N, N+1:2*N) = I;
H((N-1)*N + 1:N^2,(N-2)*N + 1:(N-1)*N) = I;
H((N-1)*N + 1:N^2,(N-1)*N + 1:N^2) = B;

H = k*H;
%% defining the potential well
A = ones(1,N);
for i = 2:N
    A(i) = 1 / ((i-1)*dx);
end
A(1) = 1 / 10^-20;

V = zeros(N^2, N^2);
for i = 1:N
    K = circshift(A, [0, (i - 1)]);
    for j = i-1:-1:1
        K(j) = 1 / ((i-j)*dx);
    end
```

```
    K = diag(K);
    V((i-1)*N + 1:(i)*N, (i-1)*N + 1:(i)*N) = K;
end

V = C*V;
%% eigensolver
H = H + V;
[WF, En] = eig(H);

%% GRAPHS
figure(p)
psi = reshape(WF(:, N^2-2), N, N);

surf(psi.^2)
%view([0 90])
xlabel('x1')
ylabel('x2')

E(p) = En(N^2, N^2);

if p == 1
    psi = reshape(WF(:, N^2), N, N);
    figure(7)
    subplot(321)
    surf(psi.^2)
    view([0 90])
    xlabel('x1')
    ylabel('x2')
    E25(1) = En(N^2, N^2);

    psi = reshape(WF(:, N^2-1), N, N);
    subplot(322)
    surf(psi.^2)
    view([0 90])
    xlabel('x1')
    ylabel('x2')
    E25(2) = En(N^2-1, N^2-1);

    psi = reshape(WF(:, N^2-2), N, N);
    subplot(323)
    surf(psi.^2)
    view([0 90])
    xlabel('x1')
    ylabel('x2')
    E25(3) = En(N^2-2, N^2-2);


    psi = reshape(WF(:, N^2-3), N, N);
    subplot(324)
    surf(psi.^2)
    view([0 90])
    xlabel('x1')
    ylabel('x2')
    E25(4) = En(N^2-3, N^2-3);
```

```
    psi = reshape(WF(:, N^2-4), N, N);
    subplot(325)
    surf(psi.^2)
    view([0 90])
    xlabel('x1')
    ylabel('x2')
    E25(5) = En(N^2-4, N^2-4);

    psi = reshape(WF(:, N^2-5), N, N);
    subplot(326)
    surf(psi.^2)
    view([0 90])
    xlabel('x1')
    ylabel('x2')
    E25(6) = En(N^2-5, N^2-5);

end

end
```