Bose-Einstein Condensation Problem in 3D

AMATH 481 Final Project Report

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I. Abstract

Bose-Einstein Condensation (BEC) is a state of matter in condensed matter physics. This state was first predicted by Albert Einstein following and crediting a pioneering paper by Satyendra Nath Bose on the filed of quantum statistics. This state is typically formed when a gas of bosons at low densities is cooled to temperatures very close to absolute zero. One of the simplifications of the BEC problem is known as the Gross-Pitaevskii equation which is a partial derivative equation (PDE). We can solve the problem in 3D by using Numerical Approach, and specifically by implementing the problem using the Spectral method with Fourier Transform.

II. Numerical Approach

To begin with the Gross-Pitaevskii equation:

$$i\psi_t + \frac{1}{2}\nabla^2\psi - |\psi|^2\psi + [A_1 sin^2(x) + B_1][A_2 sin^2(y) + B_2][A_3 sin^2(z) + B_3]\psi = 0$$

With given parameters A, B and grid X, Y, Z, the variable we need to solve is ψ and ψ_t. By using the ode45 operator in MATLAB, we can solve this PDE. Now, to make the above equation more intuitive for the following implementation, I will get ψ_t in terms of other parameters, now we can get the following equation:

$$i\psi_t = -(\frac{1}{2}\nabla^2\psi - |\psi|^2\psi + [A_1 sin^2(x) + B_1][A_2 sin^2(y) + B_2][A_3 sin^2(z) + B_3]\psi)$$

$$\Longrightarrow \psi_t = -\frac{1}{i}(\frac{1}{2}\nabla^2\psi - |\psi|^2\psi + [A_1 sin^2(x) + B_1][A_2 sin^2(y) + B_2][A_3 sin^2(z) + B_3]\psi)$$

$$\Longrightarrow \psi_t = i(\frac{1}{2}\nabla^2\psi - |\psi|^2\psi + [A_1 sin^2(x) + B_1][A_2 sin^2(y) + B_2][A_3 sin^2(z) + B_3]\psi)$$

In the above equation, i as the imaginary unit. If we look close to the equation in the bracket, we can divide it into a linear part and a nonlinear part, with:

$$lin = \frac{1}{2}\nabla^2\psi$$

$$nlin = -|\psi|^2\psi + [A_1 sin^2(x) + B_1][A_2 sin^2(y) + B_2][A_3 sin^2(z) + B_3]\psi$$

$$\psi_t = i(lin + nlin)$$

The boundary condition for this problem is periodic, so we will be implementing using the Spectral Method because it is relatively easy and very efficient considering the running time being $O\big(Nlog(N)\big)$.

III. Implementation

In MATLAB, we will first list the given parameters:

```
% List the given conditions

L = 2*pi;
n = 16;
tspan = 0:0.5:4;
A = [-1, -1, -1];
B = -A;
```

Then, we will set up the Fourier Space/Domain, the X, Y, Z grid, and Laplacian:

```
% Set up Fourier Space

kxyz = (2*pi/L)*[0:(n/2-1), (-n/2):-1];
kxyz(1) = 10^-6;
[KX, KY, KZ] = meshgrid(kxyz, kxyz, kxyz);

% Set up X, Y, Z grid

xyz2 = linspace(-L/2, L/2, n+1);
xyz = xyz2(1:n);
[X, Y, Z] = meshgrid(xyz, xyz, xyz);

% Set Laplacian

K = KX.^2 + KY.^2 + KZ.^2;
Lap = -K;
```

Next, we need to implement the rhs function, which is $\widehat{\psi_t}$ (ψ_t in Fourier Space):

```
function rhs = rhs(t, psif, A, B, X, Y, Z, n, Lap)

% Define psi in fourier space, and psi.

psif = reshape(psif, [n, n, n]);
psi = ifftn(psif);

% Linear part:

linf = (1/2).*Lap.*psif;

% Nonlinear part:

nlin_3D = (A(1).*sin(X).^2 + B(1)).*(A(2).*sin(Y).^2 +
B(2)).*(A(3).*sin(Z).^2 + B(3));
nlin = (-psi.*conj(psi) + nlin_3D).*psi;
nlinf = fftn(nlin);

% Combine linear and nonlinear part to get rhs = psift

rhs = reshape((i*(linf + nlinf)), [n^3, 1]);

end
```

After everything is set up, we can solve the problem using the ode45 operator. For this problem, we the initial conditions being cos(x)cos(y)cos(z) for Part A and sin(x)sin(y)sin(z) for Part B:

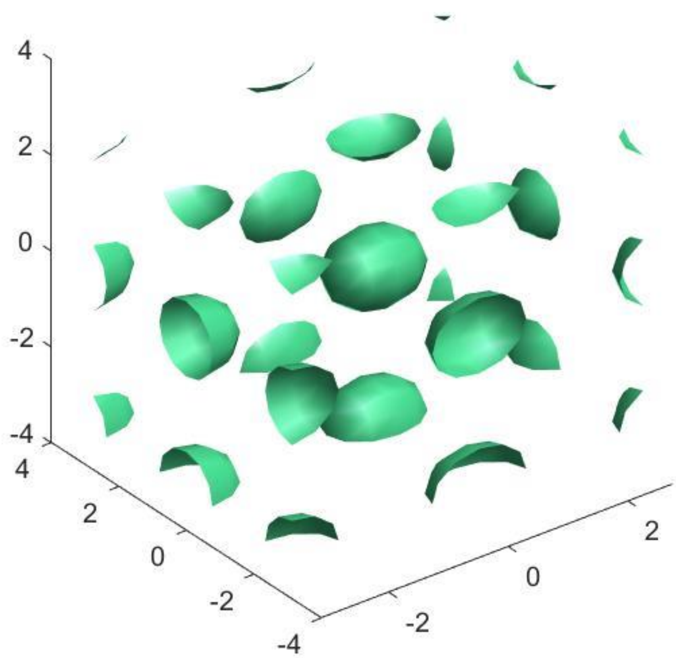
```
%% Part A: Initial Condition as cos(x)cos(y)cos(z)
% Set up initial condition

psi0 = cos(X).*cos(Y).*cos(Z);
psif0 = reshape(fftn(psi0), [n^3, 1]);

% Solve the system

[tA, psifA] = ode45(@(t, psif) rhs(t, psif, A, B, X, Y, Z, n, Lap),
tspan, psif0);

A1 = real(psifA);
A2 = imag(psifA);

%% Part B: Initial Condition as sin(x)sin(y)sin(z)
% Set up initial condition

psi0 = sin(X).*sin(Y).*sin(Z);
psif0 = reshape(fftn(psi0), [n^3, 1]);

% Solve the system

[tB, psifB] = ode45(@(t, psif) rhs(t, psif, A, B, X, Y, Z, n, Lap),
tspan, psif0);

A3 = real(psifB);
A4 = imag(psifB);
```

IV. Investigation

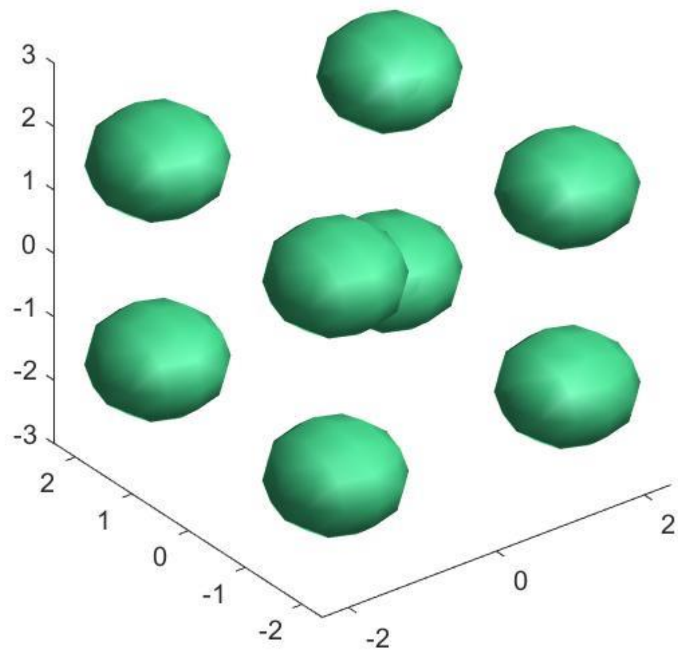
After the implementation, we can investigate the solution using MATLAB command isosurface:

```
psif = psifA;

for i = 1:size(psif, 1)

    f_cur = reshape(psif(i, :), [n, n, n]);
    cur = ifftn(f_cur);
    abscur = cur.*conj(cur);

    isosurface(X, Y, Z, abscur, 0.5);
    colormap(jet(9));
    axis('square');

end
```

We can get the following diagram for the initiation condition being cos(x)cos(y)cos(z):



Similarly, we can also get the one for the initial condition being $\sin(x)\sin(y)\sin(z)$:



From the two graphs, it makes sense for the similarity between the cosine and sine initial conditions are identical if we shift by π. We can also see that the distance and shape between the solutions at different time is very similar to each other, which implies that the system is stable. For BEC, the gas of bosons at low densities is cooled to temperature very close to absolute zero implied that it is a stable state. Hence, the symmetric shape of the two graphs makes sense for the BEC problem.