AMATH 581 Autumn Quarter 2016

Homework 6: Bose-Einstein Condensation in 3D

DUE: Wednesday, December 7, 2016 (actually Thursday, 12/8 at 3 a.m.)

Consider the Gross-Pitaevskii system (nonlinear Schrodinger with potential) modeling a condensed state of matter

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

where $\nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2$ (you can google this to learn more... or see the extra pages here). Consider periodic boundaries and using the 3D FFT (**fftn**) to solve for the evolution. Step forward using **ode45**. VISUALIZE USING **isosurface** or **slice**. WARNING: 3D problems involve working with vectors of size n^3, so pick n small to begin playing around.

ANSWERS: Let $x, y, z \in [-\pi, \pi]$, $tspan = 0 : 0.5 : 4$, $n = 16$, and parameters $A_i = -1$ and $B_j = -A_j$, with initial conditions

$$\psi(x, y, z) = \cos(x)\cos(y)\cos(z) \tag{2}$$

write out the solution of your numerical evolution from ode45 as A1.dat. (NOTE: your solution will be in the Fourier domain when your write it out.)

ANSWERS: Now solve with initial conditions

$$\psi(x, y, z) = \sin(x)\sin(y)\sin(z) \tag{3}$$

write out the solution of your numerical evolution from ode45 as A2.dat. (NOTE: your solution will be in the Fourier domain when your write it out.)

Background on BECs

To consider a specific model that allows the connection from the microscopic scale to the macroscopic scale, we examine mean-field theory of many-particle quantum mechanics with the particular application of BECs trapped in a standing light wave. The classical derivation given here is included to illustrate how the local model and its nonlocal perturbation are related. The inherent complexity of the dynamics of N pairwise interacting particles in quantum mechanics often leads to the consideration of such simplified mean-field descriptions. These descriptions are a blend of symmetry restrictions on the particle wave function and functional form assumptions on the interaction potential.

The dynamics of N identical pairwise interacting quantum particles is governed by the time-dependent, N-body Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta^N\Psi + \sum_{i,j=1,i\neq j}^{N} W(\mathbf{x}_i - \mathbf{x}_j)\Psi + \sum_{i=1}^{N} V(\mathbf{x_i})\Psi, \tag{4}$$

where $\mathbf{x_i} = (x_{i1}, x_{i2}, x_{i3})$, $\Psi = \Psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, ..., \mathbf{x}_N, t)$ is the wave function of the N-particle system, $\Delta^N = \left(\nabla^N\right)^2 = \sum_{i=1}^N \left(\partial_{x_{i1}}^2 + \partial_{x_{i2}}^2 + \partial_{x_{i3}}^2\right)$ is the kinetic energy or Laplacian operator for N-particles,

$W(\mathbf{x_i}-\mathbf{x_j})$ is the symmetric interaction potential between the i-th and j-th particle, and $V(\mathbf{x}_i)$ is an external potential acting on the i-th particle. Also, $\hbar$ is Planck's constant divided by 2π and m is the mass of the particles under consideration.

One way to arrive at a mean-field description is by using the Lagrangian reduction technique, which exploits the Hamiltonian structure of Eq. (4). The Lagrangian of Eq. (4) is given by

$$L = \int_{-\infty}^{\infty} \left\{ i\frac{\hbar}{2}\left(\Psi\frac{\partial\Psi^*}{\partial t} - \Psi^*\frac{\partial\Psi}{\partial t}\right) + \frac{\hbar^2}{2m}\left|\nabla^N\Psi\right|^2 + \sum_{i=1}^{N}\left(\sum_{j\neq i}^{N} W(\mathbf{x}_i-\mathbf{x}_j) + V(\mathbf{x}_i)\right)|\Psi|^2 \right\} d\mathbf{x}_1\cdots d\mathbf{x}_N\,. \tag{5}$$

The Hartree-Fock approximation for bosonic particles uses the separated wave function ansatz

$$\Psi = \psi_1(\mathbf{x}_1,t)\psi_2(\mathbf{x}_2,t)\cdots\psi_N(\mathbf{x}_N,t) \tag{6}$$

where each one-particle wave function $\psi(\mathbf{x}_i)$ is assumed to be normalized so that $\langle\psi(\mathbf{x}_i)|\psi(\mathbf{x}_i)\rangle^2 = 1$. Since identical particles are being considered,

$$\psi_1 = \psi_2 = \ldots = \psi_N = \psi, \tag{7}$$

enforcing total symmetry of the wave function. Note that for the case of BECs, assumption (6) is approximate if the temperature is not identically zero.

Integrating Eq. (5) using (6) and (7) and taking the variational derivative with respect to $\psi(\mathbf{x}_i)$ results in the Euler-Lagrange equation

$$i\hbar\frac{\partial\psi(\mathbf{x},t)}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi(\mathbf{x},t)+V(\mathbf{x})\psi(\mathbf{x},t)+ (N-1)\psi(\mathbf{x},t)\int_{-\infty}^{\infty}W(\mathbf{x}-\mathbf{y})|\psi(\mathbf{y},t)|^2 d\mathbf{y}. \tag{8}$$

Here, $\mathbf{x}=\mathbf{x}_i$, and Δ is the one-particle Laplacian in three dimensions. The Euler-Lagrange equation (8) is identical for all $\psi(\mathbf{x}_i,t)$. Equation (8) describes the nonlinear, nonlocal, mean-field dynamics of the wave function $\psi(\mathbf{x},t)$ under the standard assumptions (6) and (7) of Hartree-Fock theory. The coefficient of $\psi(\mathbf{x},t)$ in the last term in Eq. (8) represents the effective potential acting on $\psi(\mathbf{x},t)$ due to the presence of the other particles.

At this point, it is common to make an assumption on the functional form of the interaction potential $W(\mathbf{x}-\mathbf{y})$. This is done to render Eq. (8) analytically and numerically tractable. Although the qualitative features of this functional form may be available, for instance from experiment, its quantitative details are rarely known. One convenient assumption in the case of short-range potential interactions is $W(\mathbf{x}-\mathbf{y}) = \kappa\delta(\mathbf{x}-\mathbf{y})$ where δ is the Dirac delta function. This leads to the Gross-Pitaevskii mean-field description:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + \beta|\psi|^2\psi + V(\mathbf{x})\psi, \tag{9}$$

where $\beta = (N-1)\kappa$ reflects whether the interaction is repulsive ($\beta > 0$) or attractive ($\beta < 0$). The above string of assumptions is difficult to physically justify. Nevertheless, Lieb and Seiringer show that Eq. (9) is the correct asymptotic description in the dilute-gas limit. In this limit, Eqs. (8) and (9) are asymptotically equivalent. Thus, although the nonlocal Eq. (8) is in no way a more valid model than the local Eq. (9), it can be interpreted as a perturbation to the local Eq. (9).