MA5232 Homework and Project 1

(Due date: 6:00pm February 26, 2018 (Monday))

Consider the three-dimensional (3D) Gross-Pitaevskii equation (GPE) for modeling Bose-Einstein condensate (BEC) with a harmonic plus optical lattice potential:

$$i\hbar\frac{\partial\psi(\mathbf{x},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{x},t) + \left[V_{\mathrm{ho}}(\mathbf{x}) + V_{\mathrm{opt}}(\mathbf{x})\right]\psi(\mathbf{x},t) + g|\psi(\mathbf{x},t)|^2\psi(\mathbf{x},t), \tag{1}$$

where $\mathbf{x} = (x, y, z)^T$ is the spatial coordinate vector, t is time, $\psi = \psi(\mathbf{x}, t)$ is the macroscopic wave function, m is the atomic mass, $\hbar$ is the planck constant, $g = \frac{4\pi\hbar^2 a_s}{m}$ describes the interaction between atoms in the condensate with a_s the s-wave scattering length (positive for repulsive interaction and negative for attractive interaction). $V_{\mathrm{ho}}(\mathbf{x})$ and $V_{\mathrm{opt}}(\mathbf{x})$ are external harmonic and optical lattice trapping potentials, respectively and given as

$$V_{\mathrm{ho}}(\mathbf{x}) = \frac{m}{2}\left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right),$$

with ω_x, ω_y and ω_z trap frequencies in x-, y- and z-direction, respectively, and

$$V_{\mathrm{opt}}(\mathbf{x}) = S_0\, E_0\left[\sin^2\left(\frac{2\pi x}{\lambda_0}\right) + \sin^2\left(\frac{2\pi y}{\lambda_0}\right) + \sin^2\left(\frac{2\pi z}{\lambda_0}\right)\right],$$

with λ_0 the wavelength of the laser light creating the lattice, and $E_0 = \frac{2\pi^2\hbar^2}{m\lambda_0^2}$ the so-called recoil energy and S_0 a dimensionless constant. The macroscopic wave function ψ at time $t = 0$ is normalized at

$$\int_{\mathcal{R}^3} |\psi(\mathbf{x}, 0)|^2\, dxdydz = N, \tag{2}$$

with N the total number of atoms in the condensate.

1. Dimensionless the above GPE (1) by choosing the dimensionless time unit $t_s = \frac{1}{\omega_x}$ and $x_s = \sqrt{\frac{\hbar}{m\omega_x}}$ such that the dimensionless macroscopic wave function is normalized to unity. Using the two typical experimental parameters in the bottom, find the dimensionless time unit t_s, space unit x_s and energy unit $E_s = \frac{\hbar}{t_s} = \frac{\hbar^2}{mx_s^2}$ and express the dimensionless constants in terms of the total number of particle N in the condensate.

2. When $N \gg 1$, re-scale the above dimensionless GPE into the semiclassical form.

3. Dimensionless the above GPE (1) by choosing the dimensionless time unit $t_s = \frac{m\lambda_0^2}{4\pi^2\hbar}$ and $x_s = \frac{\lambda_0}{2\pi}$ such that the dimensionless macroscopic wave function is normalized to unity. Again, using the two typical experimental parameters in the bottom, find the dimensionless time unit t_s, space unit x_s and energy unit $E_s = \frac{\hbar}{t_s} = \frac{\hbar^2}{mx_s^2}$ and express the dimensionless constants in terms of the total number of particle N in the condensate.

4. Based on the dimensionless GPE in part 1, prove that the normalization and energy are conserved.

5. Reduce the 3D dimensionless GPE to a 2D GPE when $\omega_y \approx \omega_x$, $\omega_z \gg \omega_x$ and 1D GPE when $\omega_y \gg \omega_x$, $\omega_z \gg \omega_x$. Summarize the 1D, 2D and 3D GPE in a general form.

6. Find the approximate ground state solution of the dimensionless GPE for strong repulsive interaction (Thomas-Fermi approximation).

7. Design an imaginary time method to compute the ground state solution and develop a code to compute the ground state in 1D and 2D for different parameter regimes. Plot the ground state and the corresponding energy and chemical potential. Compare your numerical results with the Thomas-Fermi approximation. What conclusions can you get?

8. Design a time-splitting spectral method to compute the dynamics of GPE and develop a code for the the method in 1D and 2D. Use your code to study the dynamics of the GPE, with different interaction parameters and with different trapping potentials. What conclusion can you get?

9. In 1D, if we choose the initial data as

$$\psi(x,0) = \phi_g(x - x_0)\, e^{i\alpha x}, \qquad -\infty < x < \infty,$$

with $\phi_g(x)$ the ground state of the original GPE and x_0 and α given constants, study asymptotically and numerically the dynamics of the center of mass and condensate width defined as

$$\begin{aligned} x(t) &:= \langle x\rangle(t) = \int_{-\infty}^{\infty} x|\psi(x,t)|^2\, dx, \qquad t \geq 0, \\ \sigma(t) &:= \sqrt{\delta(t)} := \sqrt{\int_{-\infty}^{\infty} x^2|\psi(x,t)|^2\, dx}, \qquad t \geq 0. \end{aligned}$$

The following are two sets of physical parameters used in typical BEC experiments:

- BEC experiment with ^{87}Rb

$$\begin{aligned} &\hbar = 1.05\times 10^{-34}[J\ s], \qquad m = 1.443\times 10^{-25}[kg], \\ &\omega_x = 20\times 2\pi[1/s], \qquad \omega_y = \omega_z = 10\omega_x; \\ &a_s = 5.1[nm], \qquad \lambda_0 = 911.8[nm], \qquad S_0 = 2. \end{aligned}$$

- BEC experiment with ^{23}Na

$$\begin{aligned} &\hbar = 1.05\times 10^{-34}[J\ s], \qquad m = 3.816\times 10^{-26}[kg], \\ &\omega_x = 20\times 2\pi[1/s], \qquad \omega_y = \omega_z = 10\omega_x; \\ &a_s = 2.6[nm], \qquad \lambda_0 = 911.8[nm], \qquad S_0 = 2. \end{aligned}$$