PHY635, II-Semester 2022/23, Assignment 4 solution

(1) Dark solitons: Consider an infinitely extended homogenous BEC of atoms with mass m in one-dimension[1] having a background-density ρ and repulsive interactions with strength $U_0 > 0$ (no trap).

(a) Show that for the right choice of the parameter η and the chemical potential μ, the condensate wavefunction

$$\phi(x) = \sqrt{\rho}\tanh(x/\eta) \tag{1}$$

solves the TIGPE [4].
Hints: $\tanh(x)'' = -2\text{sech}(x)^2\tanh(x)$, $\quad \text{sech}^2(x) + \tanh^2(x) = 1$.

Solution: The TIGPE without trap is:

$$\mu\phi(x) = \Big[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U_0|\phi(x)|^2\Big]\phi(x) \tag{2}$$

First, note that for $|x| \to \infty$, the proposed $\phi(x) = \sqrt{\rho}\tanh(x/\eta)$ gives $|\phi(x)|^2 \to \rho =$ const, hence the kinetic energy term in the TIGPE for $|x| \to \infty$ is zero and we know that $\mu = U_0\rho$.

When inserting $\phi(x)$ into (2) the hints give us:

$$\mu\sqrt{\rho}\tanh(x/\eta) = \Big[\frac{2\hbar^2}{2m\eta^2}sech(x/\eta)^2 + U_0\rho|\tanh(x/\eta)|^2\Big]\sqrt{\rho}\tanh(x/\eta) \Rightarrow$$

$$\mu = \frac{\hbar^2}{m\eta^2}sech(x/\eta)^2 + U_0\rho\tanh(x/\eta)^2 \tag{3}$$

To use the second hint, we need to generate a common prefactor in both terms, which happens for

$$\eta = \frac{\hbar}{\sqrt{mU_0\rho}}. \tag{4}$$

For that choice of η we have

$$\mu = U_0\rho(sech(x/\eta)^2 + \tanh(x/\eta)^2) \overset{Hint\ 2}{=} U_0\rho, \tag{5}$$

which is true, hence the dark soliton solution $\phi(x) = \sqrt{\rho}\tanh(x/\eta)$ solves the TIGPE.

(b) Discuss the implications of the wavefunction in Eq. (1) and identify the physical meaning of the required η [2].

Solution: The wavefunction describes a density dip at $x = 0$, since

[1] Ignoring the technicality that we shouldn't have one in 1D, in practice we can still have them in a finite system that really is 3D and just strongly confined in the other two directions.

$|\phi(x)|^2 = \rho\tanh^2(x/\eta)$ vanishes there. Near zero the density drops from ρ at large distances to zero monotonously over a lengthscale of η, which we recognise as $\eta = \sqrt{2}\xi$, where ξ is the healing length. Thus the "size" of the dark soliton, is (once again) given by the healing length. We can also note that the phase of the condensate is 0 on one side of it and π on the other, the soliton thus represents a kink (or discontinuity) in the complex phase of the mean field (which is why density has to vanish at the centre).

(c) Your derivation in (a) had assumed a constant background density. Under which conditions do you think you could you still use your result in the centre of a very large harmonically trapped Thomas-Fermi BEC? If you do this, you need a relation between atom-number, trapping parameters and peak density in the BEC (without dark soliton). Find this relation in order to later apply it in Q3(c) [2].

Solution: If the size of the soliton is very small compared to the scale on which the density of the BEC varies, the solution should still be valid. Thus we need $\eta \ll R_{tf}$, where R_{tf} is the Thomas Fermi radius.

To relate the atom number and chemical potential for a 1D BEC in the Thomas Fermi approximation, we use that the atom number is

$$N = \int_{-R_{tf}}^{R_{tf}} \rho(x)dx = \int_{-R_{tf}}^{R_{tf}} \frac{\mu - \frac{1}{2}m\omega^2x^2}{U}dx = \frac{4\sqrt{2}\mu^{3/2}}{3U\omega\sqrt{m}}, \tag{6}$$

This can be solved to get μ as a function of N

$$\mu = \frac{m^{1/3}(3NU\omega)^{2/3}}{2^{5/3}}. \tag{7}$$

(d) Google the definition of the term "soliton" and discuss it in the context of your solution above [2].

Solution: We find that a soliton is a solution of a non-linear wave-equation in which dispersive and nonlinear effects exactly balance, such that the waveform can propagate without change of shape. While we have not looked at propagation in this equation, the fact that we found a solution of the TIGPE implies it being a steady state, hence it "propagates without change of shape". Here, the repulsive interactions favor the density dip, while the kinetic energy term tries to remove it, hence the two can balance

(2) Variational calculation of condensate width for weak interaction: Consider a 1D condensate with weak repulsive or attractive interactions U_0. Using the variational Ansatz:

$$\phi(x) = \sqrt{N}\frac{1}{(\pi\sigma(U_0)^2)^{1/4}}e^{-\frac{x^2}{2\sigma(U_0)^2}}, \tag{8}$$

find the optimal $\sigma(U_0)$ (σ as a function of U_0) for either sign. Discuss your result [8].

Solution:

The energy functional is given by :

$$E = \int_{-\infty}^{\infty} \phi^*(x)\Big[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{m\omega^2 x^2}{2} + \frac{U_o}{2}|\phi(x)|^2\Big]\phi(x)dx \tag{9}$$

Putting $\phi(x)$ from Eq. (8) in Eq. (9), the integral yields:

$$E(\sigma) = N\left(\frac{\hbar^2}{4m\sigma^2} + \frac{1}{4}m\omega^2\sigma^2 + \frac{1}{2\sqrt{2\pi}}\frac{U_0 N}{\sigma}\right). \tag{10}$$

We now find stationary points (including minima) of this energy, by demanding $dE(\sigma)/d\sigma = 0$, which yields the equation:

$$-\frac{\hbar^2}{2m\sigma^3} + \frac{1}{2}m\omega^2\sigma - \frac{1}{2\sqrt{2\pi}}\frac{U_0 N}{\sigma^2} = 0 \tag{11}$$

In principle, solving the above equation once for $U_o \to +U_o$ and $U_o \to -U_o$ provides us with the condensate width. Due to the multiple different powers of σ this is best done on a computer, see PS for a drawing.

(3) Numerical condensate ground states and grey soliton dynamics:

The script `Assignment4_phy635_program_draft_v2.xmds` first evolves the imaginary time GPE [Eq. (3.48)], for a certain duration of "imaginary time", followed by the real time GPE [Eq. (3.41)] for a second interval of "real time".

(a) Modify the code such that it includes a harmonic potential (use parameters provided), and give it the expected Thomas-Fermi profile for the chosen atom number and interaction constant as initial state (initial "guess" of the ground-state). You can use `check_imagtime.m` to see if the imaginary time has converged (how? why does the script plot what it plots?) and to see how the true the ground-state looks like. Try to change parameters such that the result looks more (less) "Thomas-Fermi-like". Also change your initial state into some crazy choices. Discuss what you find. [4]

Solution: See solution package for code. After getting the TF profile in a harmonic trap from the imaginary time, we just implant the soliton by multiplying the profile with $\tanh(x/\eta)$. *The trick is to use the right η, for which we can use our result from Q1(c) and then $\eta = \xi/2$, with chemical potential μ inserted into ξ.*

The basic imaginary time check is shown in Fig. 1. We plot the final result and the result half way through the chosen interval of imaginary time. Since they both match 1:1, we conclude that the imaginary time has converged (the final result no longer changes for longer duration of imaginary time). We can see that for smaller interaction strengths or smaler particle numbers, the result looks more like a Gaussian and less like a TF, with the tails at the edges growing in fractional importance. For more exotic initial states such as a step function, we see that we nontheless get the same final answer from the imaginary time evolution, albeit maybe after a

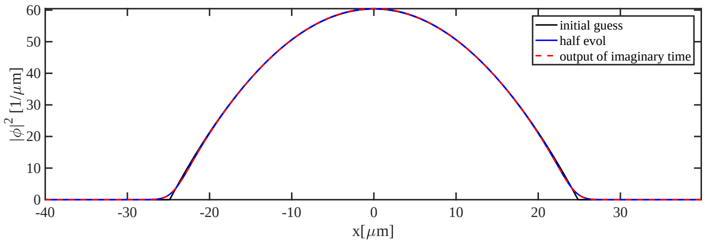

Figure 1: Output of `check_imagtime.m` for $N_{atoms} = 2000$ and $\omega/(2\pi) = 10$ Hz.

longer imaginary evolution time, and with a different looking initial imaginary time evolution.

(b) Insert your dark soliton from Q1 at $x_0 = 0$ by uncommenting the filter-block provided and modifying its content. You can now use `density_slideshow_realttimeonly_v1.m` to test your answer from Q1. Discuss. [4]

Solution: See solution codes. We patch on the soliton by multiplying $\phi(x) *= \tanh(x/\eta)$*, where* η *was found in Q1. We can use the relation from Q1c to know* $\rho(0)$ *from* ω *and* N_{atoms} *prior to starting the code, otherwise we would have to extract* $\rho(0)$ after *the imaginary time evolution and use that one in* η*. If we got it right, we see that the dark soliton remains as an almost steady state in the centre of the trap, with minor wiggles due to the fact that the background is NOT perfectly constant density. If we got the width wrong, then the width of the soliton shows oscillations in time, and the BEC will become much more disturbed.*

(c) Finally, insert your solution from Q1 at $x_0 = 0$ and then change the complex phase of the condensate wavefunction on the RHS ($x > 0$) by 0.05π, thus perturbing the system. Discuss what you find with `check_soliton_motion.m`. Discuss a few options how you could attempt to analytically understand your observations. [4]

Solution: The script extracts the position of the minimum of the density as a function of time, and results in something like Fig. 3. The steps are due to the discrete spatial gridpoints, which allow only certain positions of minima. The script had allowed to plot a sinusoidal function for comparison, with which you could have found (by trial and error) that the oscillation frequency is $\omega_{sol} = \sqrt{2}\omega$*, where* ω *is the trapping frequency.*

This results are not quite obvious, but could have been found e.g. using sophisticated variational techniques or by solving the BdG equations for a dark soliton in the centre of a harmonic trap.

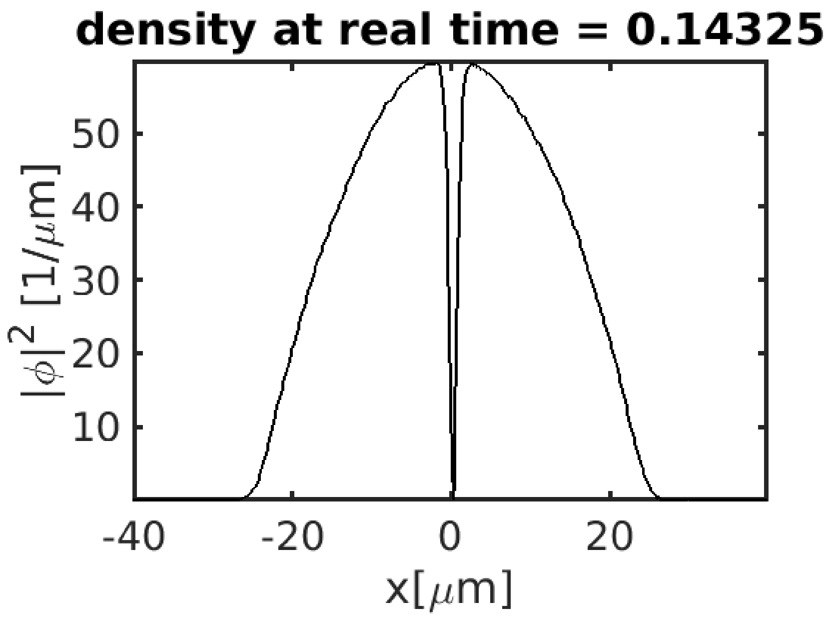

Figure 2: Output of `density_slideshow_realttimeonly_v1.m` for $N_{atoms} = 2000$ and $\omega/(2\pi) = 10$ Hz.

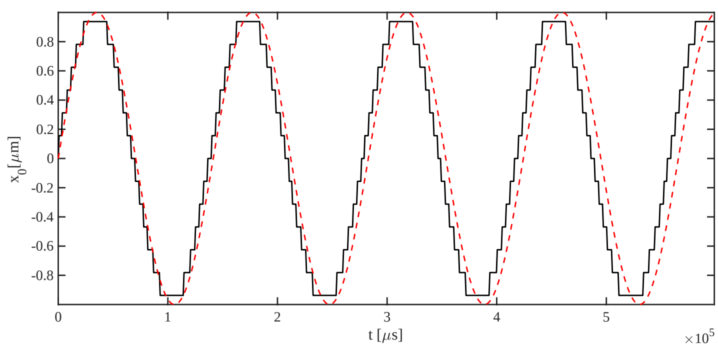

Figure 3: Dark soliton position (black) compared with $x(t) = x_0 \sin(\sqrt{2}\omega t)$, with x_0 matched into the amplitude of oscillations, and ω the trapping frequency.