PHY635, I-Semester 2019/20, Assignment 3

Instructor: Sebastian Wüster
Due-date: TA-Class, 13.9.2019

Student Name: **ID #:**

Student Name: **ID #:**

Student Name: **ID #:**

Student Name: **ID #:**

(1) Gross-Pitaevskii equation

Consider N Bosonic atoms of mass m in a 3D isotropic harmonic trap $V(\mathbf{x}) = \frac{1}{2}m\omega^2\mathbf{x}^2$ that undergo Bose-Einstein condensation.

(i) Discuss in your own words why we can use an approximate delta-function contact interaction to deal with scattering of the ultra-cold, condensed atoms, and why that is useful. [*4 points*]

(ii) Now use a field-operator $\hat{\Psi}(\mathbf{x})$ to describe these atoms, take into account contact interactions as discussed in the lecture and derive an equation of motion for the field operator $\hat{\Psi}(\mathbf{x})$. [*4 points*]

(iii) Now assume the field-operator acquires a non-vanishing expectation value upon condensation, such that $\langle\hat{\Psi}\rangle \approx \phi_0$, and find an equation from which you can obtain $\phi_0(\mathbf{x}, t)$ if you know its initial state $\phi_0(\mathbf{x}, 0)$. *You may approximate* $\langle\hat{\Psi}^\dagger\hat{\Psi}\hat{\Psi}\rangle \approx \phi_0^*\phi_0\phi_0$. [*3 points*]

(iv) Can you also reach a simple equation such as the above without the factorization assumption $\langle\hat{\Psi}^\dagger\hat{\Psi}\hat{\Psi}\rangle \approx \phi_0^*\phi_0\phi_0$? If you try to avoid that assumptions, how could you try to proceed to find equation(s) anyway? [*4 points*]

(2) Bose-Einstein condensation in varying dimensions Reconsider the derivation of Bose-Einstein condensation in section 3.2. of the lecture notes. Instead of the special example of a 3D isotropic trap, assume a generic scenario where you assume a density of states $g(E) = c_\alpha E^{\alpha-1}$.

(i) Derive the critical temperature in terms of this density of states [*5 points*]. *Hint: In the lecture we are at some point summing over all states. Note the expression only depends on the energy of these states. Assume a dense continuum of states and convert that sum into an integration, using $g(E)$. Google "density of states" if needed.*

(ii) What is the density of states in a 1D harmonic oscillator potential? [*5 points*]

(iii) Based on your results of (i) and (ii), contemplate Bose-Einstein condensation in a strictly 1D harmonic oscillator potential? [*5 points*]

Solution:

(i) *This was supposed to encourage you to think and read more about this aspect, so there is no solution. Please see Pethik and Smith and upcoming update of lecture notes.*

(ii) *The second quantized Hamiltonian for BEC is:*

$$\hat{H} = \int d\mathbf{x} \left[\hat{\mathbf{\Psi}}(\mathbf{x}) \mathbf{H_0} \hat{\mathbf{\Psi}}^\dagger(\mathbf{x}) + \frac{\mathbf{U_0}}{\mathbf{2}} \hat{\mathbf{\Psi}}^\dagger(\mathbf{x}) \hat{\mathbf{\Psi}}^\dagger(\mathbf{x}) \hat{\mathbf{\Psi}}(\mathbf{x}) \hat{\mathbf{\Psi}}(\mathbf{x}) \right],$$

The equation of motion for any operator is the Heisenberg equation. Now the Heisenberg equation for the field operator is given as:

$$\begin{aligned}
i\hbar \frac{\partial}{\partial t} \hat{\Psi}(\mathbf{x}, \mathbf{t}) &= [\hat{\Psi}(\mathbf{x}, \mathbf{t}), \hat{\mathbf{H}}] \\
&= \int d\mathbf{x}' \left[\hat{\mathbf{\Psi}}(\mathbf{x}, \mathbf{t}), \hat{\mathbf{\Psi}}(\mathbf{x}', \mathbf{t}) \mathbf{H_0} \hat{\mathbf{\Psi}}^\dagger(\mathbf{x}', \mathbf{t}) \right] \\
&+ \int d\mathbf{x}' \left[\hat{\mathbf{\Psi}}(\mathbf{x}, \mathbf{t}), \frac{\mathbf{U_0}}{\mathbf{2}} \hat{\mathbf{\Psi}}^\dagger(\mathbf{x}', \mathbf{t}) \hat{\mathbf{\Psi}}^\dagger(\mathbf{x}', \mathbf{t}) \hat{\mathbf{\Psi}}(\mathbf{x}', \mathbf{t}) \hat{\mathbf{\Psi}}(\mathbf{x}', \mathbf{t}) \right] \\
&= \int d\mathbf{x}' \hat{\mathbf{\Psi}}(\mathbf{x}', \mathbf{t}) \mathbf{H_0} \left[\hat{\mathbf{\Psi}}(\mathbf{x}, \mathbf{t}), \hat{\mathbf{\Psi}}^\dagger(\mathbf{x}', \mathbf{t}) \right] \\
&+ \frac{U_0}{2} \int d\mathbf{x}' \hat{\mathbf{\Psi}}^\dagger(\mathbf{x}', \mathbf{t}) \left[\hat{\mathbf{\Psi}}(\mathbf{x}, \mathbf{t}), \hat{\mathbf{\Psi}}^\dagger(\mathbf{x}', \mathbf{t}) \right] \hat{\mathbf{\Psi}}(\mathbf{x}', \mathbf{t}) \hat{\mathbf{\Psi}}(\mathbf{x}', \mathbf{t}) \\
&+ \frac{U_0}{2} \int d\mathbf{x}' \left[\hat{\mathbf{\Psi}}(\mathbf{x}, \mathbf{t}), \hat{\mathbf{\Psi}}^\dagger(\mathbf{x}', \mathbf{t}) \right] \hat{\mathbf{\Psi}}^\dagger(\mathbf{x}', \mathbf{t}) \hat{\mathbf{\Psi}}(\mathbf{x}', \mathbf{t}) \hat{\mathbf{\Psi}}(\mathbf{x}', \mathbf{t}) \\
&= \int d\mathbf{x}' \hat{\mathbf{\Psi}}(\mathbf{x}', \mathbf{t}) \mathbf{H_0} \delta(\mathbf{x} - \mathbf{x}') + \frac{\mathbf{U_0}}{\mathbf{2}} \int \mathbf{d}\mathbf{x}' \hat{\mathbf{\Psi}}^\dagger(\mathbf{x}', \mathbf{t}) \delta(\mathbf{x} - \mathbf{x}') \hat{\mathbf{\Psi}}(\mathbf{x}', \mathbf{t}) \hat{\mathbf{\Psi}}(\mathbf{x}', \mathbf{t}) \\
&+ \frac{U_0}{2} \int d\mathbf{x}' \delta(\mathbf{x} - \mathbf{x}') \hat{\mathbf{\Psi}}^\dagger(\mathbf{x}', \mathbf{t}) \hat{\mathbf{\Psi}}(\mathbf{x}', \mathbf{t}) \hat{\mathbf{\Psi}}(\mathbf{x}', \mathbf{t}) \\
i\hbar \frac{\partial}{\partial t} \hat{\Psi}(\mathbf{x}, \mathbf{t}) &= H_0 \hat{\Psi}(\mathbf{x}, \mathbf{t}) + \mathbf{U_0} \hat{\mathbf{\Psi}}^\dagger(\mathbf{x}, \mathbf{t}) \hat{\mathbf{\Psi}}(\mathbf{x}, \mathbf{t}) \hat{\mathbf{\Psi}}(\mathbf{x}, \mathbf{t}) \qquad (1)
\end{aligned}$$

(iii) *Taking the expectation value of Eq. (1) over the unknown many-body state gives*

$$i\hbar \frac{\partial}{\partial t} \langle \hat{\Psi}(\mathbf{x}, \mathbf{t}) \rangle = H_0 \langle \hat{\Psi}(\mathbf{x}, \mathbf{t}) \rangle + \mathbf{U_0} \langle \hat{\mathbf{\Psi}}^\dagger(\mathbf{x}, \mathbf{t}) \hat{\mathbf{\Psi}}(\mathbf{x}, \mathbf{t}) \hat{\mathbf{\Psi}}(\mathbf{x}, \mathbf{t}) \rangle.$$

You were given the hint to use $\langle \Psi \rangle = \phi_0$ *and* $\langle \hat{\Psi}^\dagger(\mathbf{x}, \mathbf{t}) \hat{\mathbf{\Psi}}(\mathbf{x}, \mathbf{t}) \hat{\mathbf{\Psi}}(\mathbf{x}, \mathbf{t}) \rangle \approx \phi_{\mathbf{0}}^* \phi_{\mathbf{0}} \phi_{\mathbf{0}}$. *Note that to use this, you don't necessarily need to know the state. In this case we don't. The statement will be true for some states, false for others, but at least a good approximation for some of the latter. Using it we find*

$$i\hbar \frac{\partial}{\partial t} \phi_0(\mathbf{x}, \mathbf{t}) = \mathbf{H_0} \phi_{\mathbf{0}}(\mathbf{x}, \mathbf{t}) + \mathbf{U_0} |\phi_{\mathbf{0}}(\mathbf{x}, \mathbf{t})|^{\mathbf{2}} \phi_{\mathbf{0}}(\mathbf{x}, \mathbf{t}).$$

(iv) Without the approximation we don't reach a simple form. We could continue by finding an equation of motion for the product *operator* $\hat{\Psi}^\dagger(\mathbf{x},\mathbf{t})\hat{\mathbf{\Psi}}(\mathbf{x},\mathbf{t})\hat{\mathbf{\Psi}}(\mathbf{x},\mathbf{t})$*. This could proceed in the same way as before, using the Heisenberg equation. The result will require equations for even more complicated operators. Nonetheless this approach (roughly) will be covered later in week 8 of the lecture.*

(2) Bose-Einstein condensation in varying dimensions *Reconsider the derivation of Bose-Einstein condensation in section 3.2. of the lecture notes. Instead of the special example of a 3D isotropic trap, assume a generic scenario where you assume a density of states* $g(E) = c_\alpha E^{\alpha-1}$.

(i) Derive the critical temperature in terms of this density of states [5 points]. Hint: In the lecture we are at some point summing over all states. Note the expression only depends on the energy of these states. Assume a dense continuum of states and convert that sum into an integration, using $g(E)$*. Google "density of states" if needed.*

(ii) What is the density of states in a 1D harmonic oscillator potential? [5 points]

(iii) Based on your results of (i) and (ii), contemplate Bose-Einstein condensation in a strictly 1D harmonic oscillator potential? [5 points]

Solution:

(i) The transition temperature T_c *is defined as the highest temperature at which the macroscopic occupation of the lowest-energy state appears. The number of particles in excited states is given as:*

$$N_{exc} = \int_0^\infty dE g(E) m(E), \tag{2}$$

where $m(E) = \frac{1}{e^{(E-\mu)/kT}-1}$ *is the mean occupation number of the single-particle state. This achieves its greatest value for* $\mu = 0$ *and the transition temperature is determined by the condition that the total number of particles can be accommodated in the excited states, that is*

$$\begin{aligned} N = N_{exc}(T_c, \mu = 0) &= \int_0^\infty dE g(E) \frac{1}{e^{E/kT_c}-1} \\ &= \int_0^\infty dE c_\alpha E^{\alpha-1} \frac{1}{e^{E/kT_c}-1} \end{aligned} \tag{3}$$

The above equation can be written in the terms of a new dimensionless variable

$x = E/kT_c$ as:

$$\begin{aligned} N &= c_\alpha (kT_c)^\alpha \int_0^\infty dx \frac{x^{\alpha-1}}{e^x - 1} \\ &= c_\alpha (kT_c)^\alpha \int_0^\infty dx \frac{e^{-x} x^{\alpha-1}}{1 - e^{-x}} \\ &= c_\alpha (kT_c)^\alpha \int_0^\infty dx e^{-x} x^{\alpha-1} \{1 + e^{-x} + e^{-2x} + \cdots\} \\ &= c_\alpha (kT_c)^\alpha \Gamma(\alpha)\zeta(\alpha), \end{aligned} \tag{4}$$

where $\Gamma(\alpha) = \int_0^\infty dx x^{\alpha-1} e^{-x}$ is Gamma function and $\zeta(\alpha) = \sum_{n=1}^\infty n^{-\alpha}$ is Riemann zeta function. Now from Eq. (4) the transition temperature can be written as:

$$kT_c = \frac{N^{1/\alpha}}{[c_\alpha \Gamma(\alpha)\zeta(\alpha)]^{1/\alpha}} \tag{5}$$

(ii) *The energy of 1D harmonic oscillator is given as:*

$$E = \hbar\omega(n + \frac{1}{2}). \tag{6}$$

For energies large compared with $\hbar\omega$, we may treat the n as a continuous variables and neglect zero point energy. The number of states $\Sigma(E)$ with energy less than a given energy E is given as:

$$\begin{aligned} \Sigma(E) &= \frac{1}{\hbar\omega} \int_0^E dE \\ &= \frac{E}{\hbar\omega} \end{aligned} \tag{7}$$

Now the density of states is given as:

$$\begin{aligned} g(E) &= \frac{d\Sigma(E)}{dE} \\ &= \frac{1}{\hbar\omega} = const. \end{aligned} \tag{8}$$

(iii) *To phrase (8) in terms of part (i), we have $\alpha = 1$ and $c_\alpha = \frac{1}{\hbar\omega}$. Thus using Eq. (5) we find $T_c = 0$ (e.g. using the Limit function in mathematica). Thus there is <u>no condensation</u> in a 1D system.*

(3) Numerical Solution of Gross-Pitaevskii equation

The attached template file `Assignment3_phy635_program_draft_v1.xmds` is set up to first find a ground-state of the Schrödinger equation with a method called "imaginary time *evolution"(see towards end of week 6), and then evolve that state in time. The ground-state finding uses a harmonic trap with frequency ω_{ini} the time evolution uses ω_{fin}.*

(4a) First test with **`density_slideshow_v1.m`** *that for $\omega_{ini} = \omega_{fin}$ the "imaginary time evolution" converges to the ground-state despite the silly initial state and the state found later does not change in real time [2 points]. Hint: note the first 101 time-samples are from the imaginary time evolution, the last 100 from the real time, the script knows this.*

(4b) Now slightly change ω_{fin} such that $\omega_{fin} \neq \omega_{ini}$. What happens? Use **`plot_widths_v1.m`** *to plot the time evolution of the position uncertainty $\Delta\hat{x}$. Quantify what you see and compare with the final harmonic trap frequency. [2 points]*

(4c) Change everything in the script that needs changing in order to tackle the Gross-Pitaevskii equation with the same traps, but 1000 atoms instead of one. Instead of U_0 from equation (4.8) we shall use an effective 1D interaction strength U_{1d} that is already defined in the code. [2 points]

(4d) Redo the same as steps (a) and (b) for the Bose-Einstein condensate and discuss your findings. Use a couple of different ω_{fin} and try to deduce a law for what you see. [4 points]

Solution:

(a) *The imaginary time evolution of the initial state for a particle in a harmonic trap is shown in Fig. 1. The final state at t* $= 0.038$ *will remain same in the real time evolution under the condition $\nu_{ini} = \nu_{fin}$.*

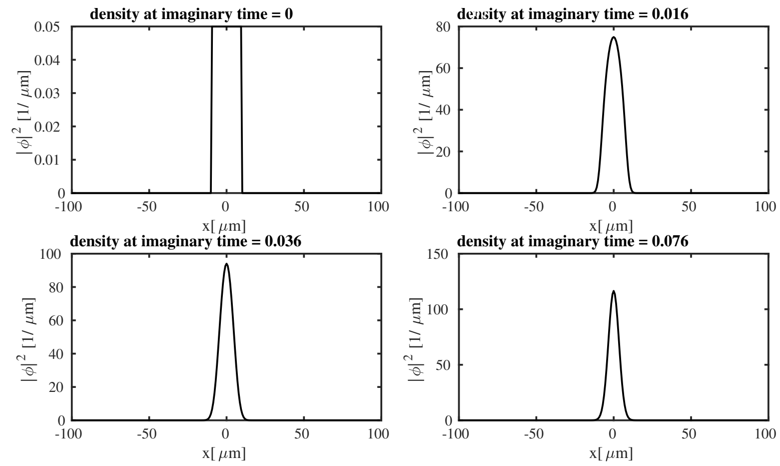

Fig. 1. The imaginary time evolution of density for $\nu_{ini} = \nu_{fin} = 5.00$.

(b) *For the case $\nu_{ini} \neq \nu_{fin}$, the density starts oscillating in the real time evolution (Fig. 2). This is called "breathing mode". The frequency of the oscillation can be calculated by counting the number of cycle in the position uncertainity, see Fig. 3. We can estimate from the figure that two breathing periods take about 0.1 s, so breathing happens at twice the trap frequency.*

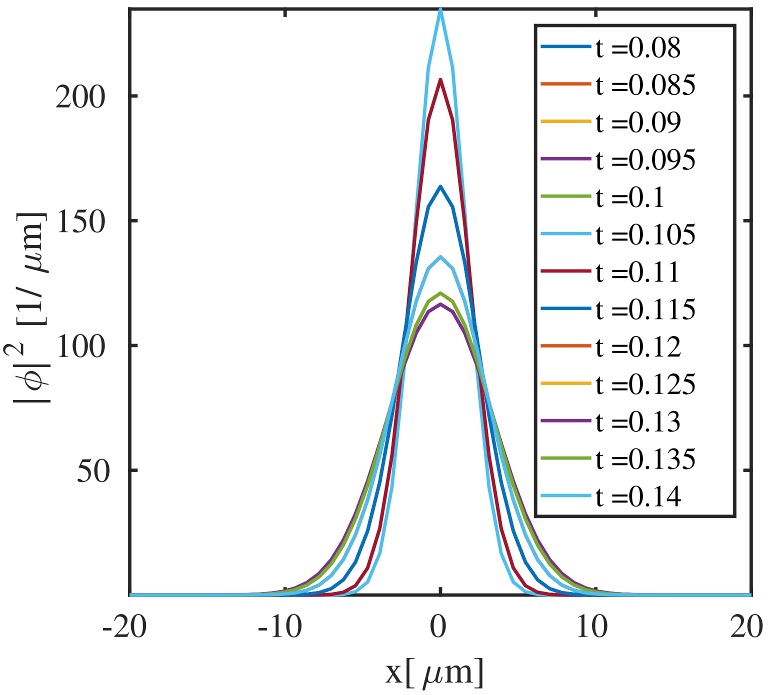

Fig. 2. Real time evolution of the density under the condition $\nu_{ini}(=5) \neq \nu_{fin}(=10)$

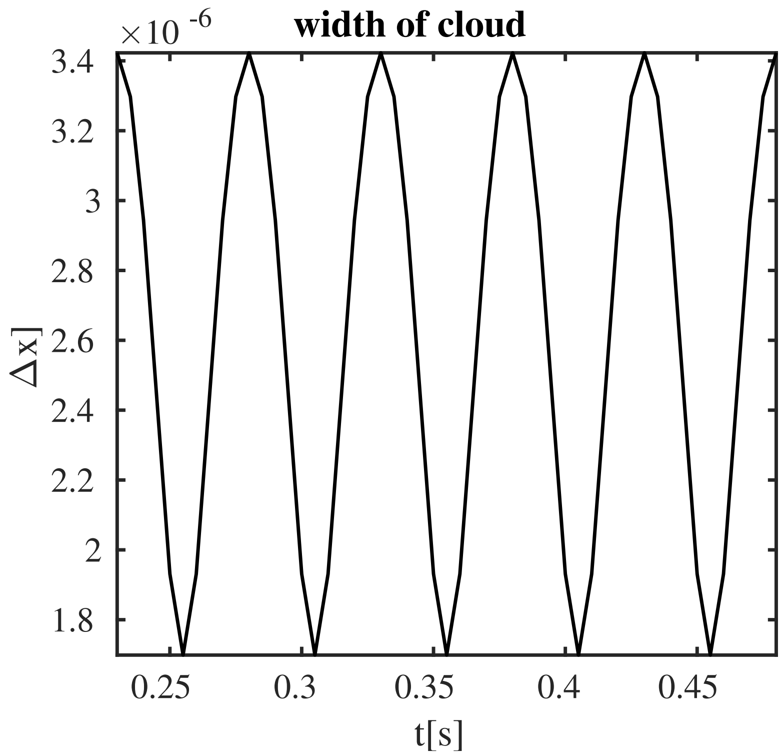

Fig. 3. Evolution of expectation value for $\nu_{ini}(=5) \neq \nu_{fin}(=10)$.

(d) Fig. 4 shows the density profile under the imaginary time evolution of the BEC for 1000 particles in a trap. The final state is achieved at $t = 0.038$ *starting with a*

completely different initial state what we had for one particle in the trap.
The real time evolution of the density profile is shown in Fig. 5 under the condition $\nu_{ini} \neq \nu_{fin}$.

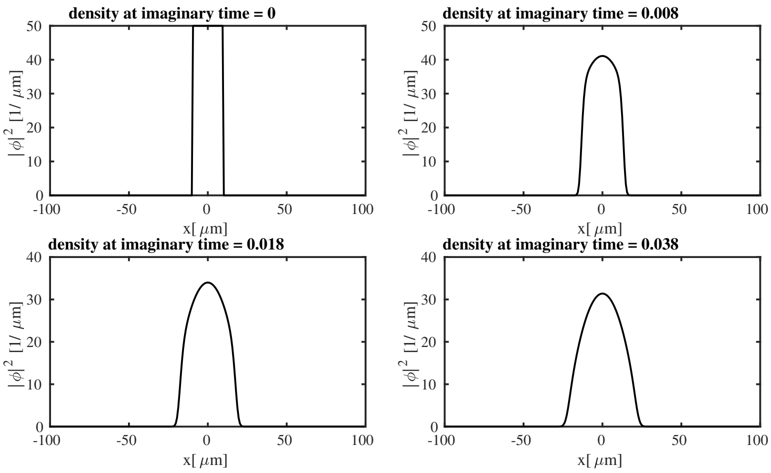

Fig. 4. The imaginary time evolution of density for BEC under the condition $\nu_{ini} = \nu_{fin} = 5.00$.

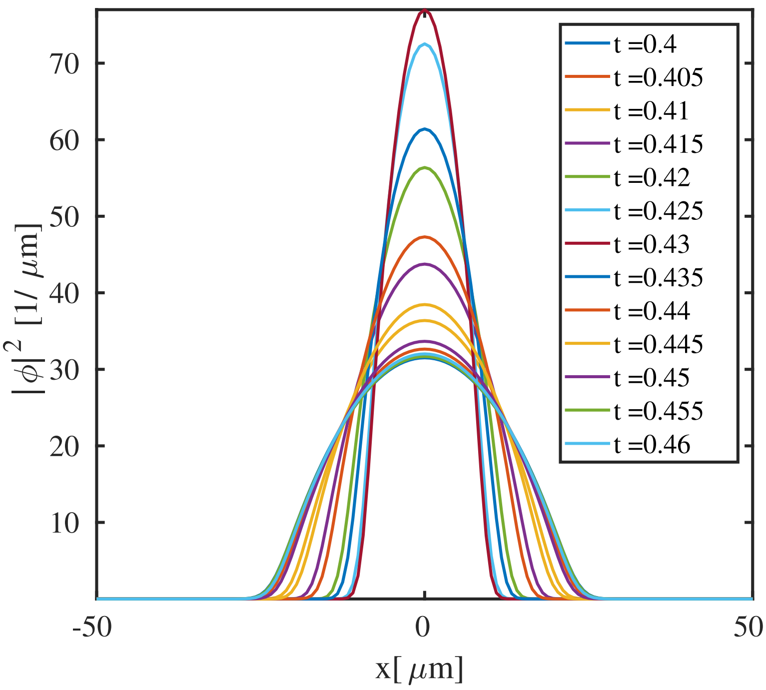

Fig. 5. The real time evolution of density for BEC cloud under the condition $\nu_{ini}(= 5) \neq \nu_{fin}(= 10)$.

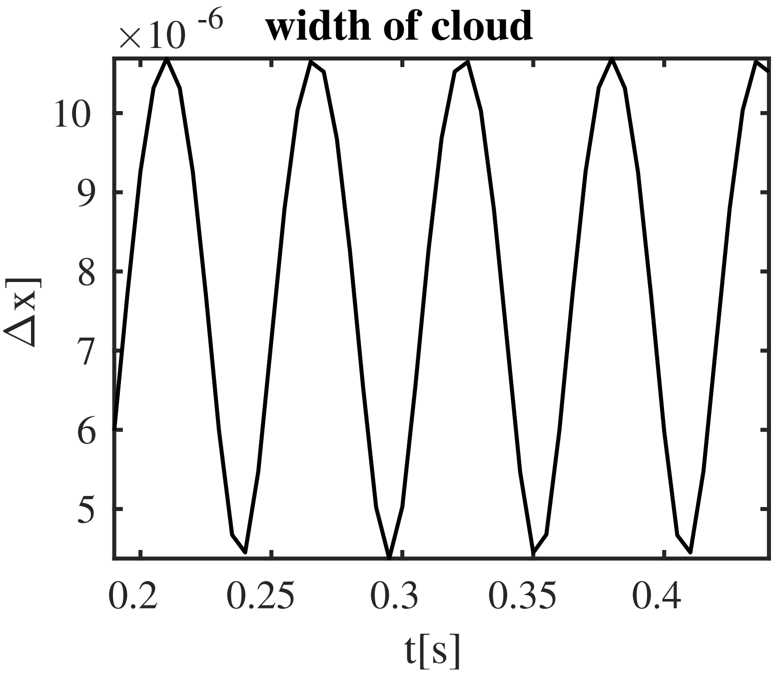

Fig. 6. Evolution of expectation value for BEC cloud under the condition $\nu_{ini}(=5) \neq \nu_{fin}(=10)$.