Inverse population transfer of the repulsive Bose-Einstein condensate in a double-well trap: strong interaction-induced support

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An inverse population transfer of the repulsive Bose-Einstein condensate (BEC) in a weakly bound double-well trap is explored within the 3D time-dependent Gross-Pitaevskii equation. The model avoids numerous common approximations (two-mode treatment, time-space factorization, etc) and closely follows the conditions of Heidelberg experiments, thus providing a realistic description of BEC dynamics. The transfer is driven by a time-dependent shift of a barrier separating the left and right wells. It is shown that completeness and robustness of the process considerably depend on the amplitude and time profile of the shift velocity. Soft profiles provide the most robust inversion. The repulsive interaction substantially supports the transfer making it possible i) in a wide velocity interval and ii) three orders of magnitude faster than in the ideal BEC.

I. INTRODUCTION

The population inversion is a typical problem met in various branches of physics (ultracold gases and condensates\textsuperscript{[1]–2}, atomic and molecular physics\textsuperscript{[3]–4}, etc.). The problem is easily solvable, if it is linear and accepts an adiabatic evolution, see e.g. the Landau-Zener scenario\textsuperscript{[5, 6]}. However, if there are significant nonlinear effects or/and we need a rapid but robust transfer, the problem becomes nontrivial, e.g. for a transport of Bose-Einstein condensate (BEC)\textsuperscript{[7, 8]}. The inverse population transfer of a repulsive BEC in a double-well trap is the relevant example of such a complex problem\textsuperscript{[8]}: the repulsive interaction in BEC leads to a strong nonlinearity and a limited life-time of BEC requests a rapid transfer. However, a rapid process, if not specially designed, is usually spoiled by dipole oscillations at the final state. The question is how to produce a robust (without final dipole oscillations) and rapid nonlinear population inversion (NLPI) in this case? Another important aspect is how does the nonlinearity affect the process?

In principle, this problem is a subject of so-called shortcuts-to-adiabaticity (StA) methods which have made a significant progress over the last years, see\textsuperscript{[2]} for an extensive review. However, to our knowledge, these methods have not yet been derived for our particular case: NLPI for BEC in a double-well trap. Moreover, even though some StA methods, like the optimal control theory\textsuperscript{[9, 10]}, may be potentially implemented in this case, their protocols might be too complicated and parameter-sensitive to be realized in experiment, while we need a simple prescription with a minimal number of control parameters. We will show that such a prescription can be built using the setup of Heidelberg experiments\textsuperscript{[1]} where a time-dependent shift $x_0(t)$ of the barrier is used as a suitable control parameter driving the trap asymmetry and thus the population transfer.

In the present study, the barrier shift is used to produce NLPI of BEC in a double-well trap. The calculations are performed within the three-dimensional (3D) time-dependent Gross-Pitaevskii equation\textsuperscript{[11]} for the total order parameter covering both left and right parts of the condensate. Our model\textsuperscript{[12]} is free from numerous approximations (two-mode treatment, time-space factorization of the order parameter, etc) widely used in investigation of BEC dynamics in a double-well trap (see e.g.\textsuperscript{[8]} and references therein) and closely follows prescriptions of the Heidelberg’s experiments\textsuperscript{[12, 13]}, thus providing quite realistic picture.

The NLPI is explored for different magnitudes and time profiles of the transfer velocity, thus covering adiabatic and rapid scenarios. Both ideal and repulsive BECs are considered to estimate the nonlinear effect caused by the interaction between BEC atoms. As shown below, the repulsive interaction strongly favours the NLPI. This is in agreement with our previous results obtained within less involved model\textsuperscript{[8]}.

The paper is organized as follows. The calculation scheme is sketched in Sec. II the results are discussed in Sec. III the summary is done in Sec. IV.

II. CALCULATION SCHEME

We use the 3D time-dependent Gross-Pitaevskii equation (GPE)\textsuperscript{[11]}

$$i\hbar \frac{\partial \Psi(r,t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r,t) + g_0|\Psi(r,t)|^2 \right] \Psi(r,t) \quad (1)$$

for the total order parameter $\Psi(r,t)$ describing the BEC in both left and right wells of the trap. Here $g_0 = 4\pi\hbar^2a_s/m$ is the interaction parameter, $a_s$ is the scatter-
The trap potential

\[ V(r, t) = V_{\text{con}}(r) + V_{\text{bar}}(x, t) = \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) + V_0 \cos^2(\pi(x - x_0(t))/q_0) \]

includes the anisotropic harmonic confinement and the barrier in \( x \)-direction, whose position is driven by the control parameter \( x_0(t) \). Furthermore, \( V_0 \) is the barrier height and \( q_0 \) determines the barrier width.

Following the Heidelberg experiment [13, 14] for measuring Josephson oscillations (JO) and macroscopic quantum self-trapping (MQST), we consider the BEC of N=1000 \(^{87}\text{Rb} \) atoms with \( a_s = 5.75 \text{ nm} \). The trap frequencies are \( \omega_x = 2\pi \times 78 \text{ Hz} \), \( \omega_y = 2\pi \times 66 \text{ Hz} \), \( \omega_z = 2\pi \times 90 \text{ Hz} \), i.e., \( \omega_y + \omega_z = 2\omega_x \). The barrier parameters are \( V_0 = 420 \times h \text{ Hz} \) and \( q_0 = 5.2 \mu m \). For the symmetric trap (\( x_0(t) = 0 \)), the distance between the centers of the left and right wells is \( d = 4.4 \mu m \). This setup has been previously used in our exploration of JO/MQST in weak and strong coupling regimes [12].

The static solutions of GPE are found within the damped gradient method [13] while the time evolution is computed within the time-splitting [16] and fast Fourier-transformation techniques. The total order parameter \( \Psi(r, t) \) is determined in a 3D cartesian grid. The requirement \( \int_{-\infty}^{\infty} dr^3|\Psi(r, t)|^2 = N \) in time is directly fulfilled by using an explicit unitary propagator. Reflecting boundary conditions are used, though they have no impact on the dynamics because the harmonic confinement makes them effectless. No time-space factorization of the parameters is used. The conservation of the total energy \( E \) and complete number of atoms \( N \) is perfectly controlled.

The populations of the left (L) and right (R) wells are computed as

\[ N_j(t) = \int_{-\infty}^{+\infty} dr^3|\Psi_j(r, t)|^2, \]

with \( J = L, R \), \( \Psi_L(R)|t) = \Psi(x \leq 0, y, z; t), \Psi_R(r, t) = \Psi(x \geq 0, y, z; t) \) and \( N_L(t) + N_R(t) = N \). The normalized population imbalance is \( z(t) = (N_L(t) - N_R(t))/N \).

The population inversion means that BEC population characterized at the initial time \( t=0 \) by \( N_{L}(0) > N_{R}(0) \) is changed during the time interval \( T \) to the inverse population \( N_{L}(T) < N_{R}(T) \) where \( N_{L}(T) = N_{R}(0) \) and \( N_{R}(T) = N_{L}(0) \).

Following the technique of [13, 14], the initial stationary asymmetric BEC state is produced by keeping the barrier right-shifted from the symmetric case \( (x(0) > 0) \). The value of the shift is adjusted to provide the given initial populations \( N_L(0) \) and \( N_R(0) \). The population inversion is generated by the time-dependent left shift of the barrier from \( x(0) \) to \( x(T) = x(0) \) with the velocity \( v(t) \). Thus asymmetry of the double-well trap is changed to the opposite one.

The quality of the inversion is characterized by its completeness \( P = -z(T)/z(0) \) (the ratio of the final and initial population imbalance) and noise \( n = A_d/N \) where \( A_d \) is amplitude of dipole oscillations in the final state, i.e., \( A_d = \max\{N_{L,R}\} - \min\{N_{L,R}\} \) for \( t > T \).

Two velocity time profiles are used: i) the sharp rectangular one with the constant \( v_c(t) = v_0^c \) at \( 0 < t < T \) and \( v_c(t) = 0 \) beyond the transfer time and ii) the soft one \( v_c(t) = v_0^c \cos^2(\frac{\pi}{2} + \frac{\pi}{2}t) \) with \( v_c(0) = v_c(T) \approx 0 \). For the total barrier shift \( D = 2x(0) \) in the inversion process of duration \( T \), the velocity amplitudes are \( v_0^c = v_0^d = D/T \). The profile \( v_c(t) \) is simple. However, it sharply changes from 0 to \( v_0^c \) at \( t=0 \) and \( T \) and so is not adiabatic. The second profile \( v_d(t) \) is more complicated but softer and thus closer to an adiabatic case.

The transfer time \( T \) has natural lower and upper limits. It cannot be longer than the BEC lifetime (\( \sim 3 \) sec). Also it cannot be too short since then the transfer would be too sharp and cause in the final state large undesirable dipole oscillations (see discussion in the next section). The same reasons determine the upper and lower limits for the transfer velocities.

### III. RESULTS AND DISCUSSION

Figure 1 exhibits the trap potential in \( x \)-direction,

\[ V_x(x, t) = \frac{m}{2}\omega_x^2 x^2 + V_0 \cos^2(\pi(x - x_0(t))/q_0), \]

calculated for the initial \( t=0 \), intermediate \( t=T/2 \) and final \( t=T \) times of the inversion process driven by the barrier shift \( x_0(t) \) with \( t \in [0,T] \). For the same times, the BEC density in \( x \)-direction,

\[ \rho(x, t) = \int_{-\infty}^{+\infty} dydz|\Psi(x, y, z, t)|^2, \]

obtained for an adiabatic inversion of a long duration \( T \) is shown. The ideal and repulsive BECs with \( N=1000 \) atoms are considered. Following the plots a) and d), the initial populations of the left and right wells are \( N_L(0)=800 \) and \( N_R(0)=200 \), i.e. with the initial population imbalance \( z(0)=0.6 \). An adiabatic evolution provides a robust population inversion to final \( N_L(T)=200 \), \( N_R(T)=800 \) and \( z(T)=0.6 \). At the intermediate time \( t=T/2 \), the trap and populations are symmetric. The initial state is stationary by construction. The intermediate and final states, if obtained adiabatically, may be also treated as stationary.

Upper plots of Fig. 1 show that for getting the initial \( z(0)=0.6 \) in the ideal BEC, a small trap asymmetry with \( x_0(0)=0.003 \mu m \) is sufficient. The overlap of the left and right parts of the condensate at the center of the trap is very small and corresponds to the case of a weak coupling. The energy difference between the ground and first excited states at the mid of the transfer (plot b)) is
\[ \Delta E(T/2) = 0.005 \hbar \text{kHz}. \] Such a tiny value confirms that the coupling and corresponding barrier penetrability are indeed small.

For the repulsive BEC (bottom plots), the initial \( N_L(0) = 800 \) and \( N_R(0) = 200 \) are obtained at much larger asymmetry with \( x_0(0) = 0.5 \mu \text{m} \). The energy splitting \( \Delta E(T/2) \) reaches 0.036 \( \hbar \text{kHz} \). This is because the repulsive interaction significantly increases the chemical potential \( \mu \) of the system and thus the coupling between the left and right parts of BEC. Then, to get the initial stationary population imbalance \( z(0) = 0.6 \), one should weaken the coupling by considerably increasing the asymmetry. As compared to the ideal BEC, the repulsive condensate has wider density bumps with much stronger overlap at the center of the trap. The coupling between the left and right BEC parts is not yet weak anymore. Nevertheless, the NLPI described below has occurred through tunneling.

Some examples of the time evolution of the populations \( N_{L,R}(t) \) in the ideal BEC (no interaction) are given in Fig. 2. The evolution is driven by the barrier shift with the rectangular \( v_c(t) \) (upper plot) and soft \( v_c(t) \) (bottom plots) velocity profiles. The total shift is \( D = 2x_0(0) = 6 \mu \text{m} \). For each example, the velocity amplitudes \( v_0^L \) and \( v_0^R \) obtained for a given transfer duration \( T \) are indicated. It is seen that, at low velocities (plots a,c)) corresponding to a long duration \( T = 1.8 \mu \text{s} \), we get rather robust population inversion. This transfer is close to an adiabatic evolution. The final state is about stationary for \( v_c(t) \) and somewhat spoiled by dipole oscillations for \( v_c(t) \). The latter is caused by the sharp change of \( v_c(t) \) from 0 to \( v_c(0) \) and back at the beginning and end of the process. In this sense, the \( v_c(t) \)-transfer is much softer and thus more adiabatic. Fig. 2 also shows that the barrier-shift technique may be used not only for the population inversion (plots a,c)) but also for production of MQST (plot b)) and JO (plot d)) supplementing the process. In our task, the JO/MQST come as undesirable dipole oscillations.

In Fig. 3, similar examples are presented for the repulsive BEC. At first glance, the non-linear evolution resembles the linear one given in Fig. 2 except for plot d)) where the final state converges to a symmetric form with \( N_L(T) \approx N_R(T) \approx 500 \) or \( z(T) \approx 0 \). Like in the linear case, a slow transfer (plots a,c)) results in a robust NLPI while a faster process (plots b,d)) spoils the final state by dipole oscillations (plot b)) or even breaks the inversion at all (plot d)). However, the nonlinearity drastically changes rates of the process. Now the robust NLPI can be produced at much shorter time \( T = 250 \mu \text{s} \) instead of \( T = 1800 \mu \text{s} \) for ideal BEC) and much faster velocities \( (\mu \text{s} \text{ instead of nms}^{-1}) \). So, despite the NLPI requires much stronger asymmetry and longer barrier shift (1 \( \mu \text{m} \) against 0.006 \( \mu \text{m} \) for the ideal BEC), the process becomes much faster. Namely, the velocities become about three order of magnitude higher (!), i.e. far beyond the adiabatic case. Therefore the repulsive interaction greatly favours the population inversion and this effect is indeed huge. The reason of the effect is simple. As mentioned above, the repulsive interaction significantly enhances the chemical potential \( \mu \), which in turn results in a dramatic increase of the barrier penetrability. The coupling between BEC fractions becomes strong and the inversion is realized much faster.

![FIG. 1: The double-well trap potential \( V_x(x) \) (bold curve) and BEC density \( \rho_x(x) \) (dash curve) at initial \( t = 0 \), intermediate \( t = T/2 \) and final inverse \( t = T \) states of the adiabatic inversion, calculated without (upper plots) and with (bottom plots) the repulsive interaction between BEC atoms. In both cases, the initial populations of the left and right wells are \( N_L(0) = 800 \) and \( N_R(0) = 200 \).](image-url)
A more general information on the robustness of the population inversion is presented in Figs. 4 and 5 where the completeness \( P \) and noise \( n \) of the inversion are illustrated for a wide range of velocity amplitudes. The inversions for the ideal and repulsive BEC are compared. In Fig. 4, the sharp velocity profile \( v_c(t) \) is used. Following the plots a) .c) for the ideal BEC, a complete inversion \( (P=1) \) takes place only at a small velocity \( v_0^c < 0.04 \) \( \mu m/s \). The inversion is somewhat spoiled by a weak noise \( n = 0.02 - 0.04 \). The smaller the velocity, the weaker the noise. For \( v_0^c > 0.04 \) \( \mu m/s \), we see a gradual destruction of the inversion, accompanied by an enhanced noise. For even larger velocities, the inversion breaks down \( (P \to 0) \) and the final state is characterized by strong Rabi oscillations \( (n \to 0.4) \). The latter effect is caused by the instant change of the process velocity from zero to \( v_0^c \) at \( t=0 \) and back at \( t=T \).

Following Fig. 4 b), the inclusion of the repulsive interaction drastically changes the results. There appears a wide plateau, \( 0 < v_0^c \leq 19 \) \( \mu m/s \), with about complete inversion \( P \approx 1 \). The repulsive interaction thus allows to get the inversion in a much wider velocity interval and, what is important, about three order of magnitude (!) faster than for the ideal BEC. Following our estimations, this is mainly caused by a considerable increase of the chemical potential \( \mu \), caused by the repulsive interaction, and thus increasing the barrier penetrability. Note that the nonlinearity plays here an important but auxiliary role, which is reduced to a mechanism of rising the chemical potential. The net effect should depend on the form of the barrier. It should be strong for barriers whose penetrability increases with the excitation energy (e.g. Gaussian and \( \cos^2(\pi x - x_0(t))/\gamma_0^2 \) barrier shapes) and suppressed for barriers with an energy-independent penetrability (e.g. rectangular shape).

The plot Fig. 4 b) exhibits a noise (Rabi oscillations at the final state) in both inversion \( v_0^c \leq 19 \) \( \mu m/s \) and beyond \( v_0^c \geq 19 \) \( \mu m/s \) regions. In the former region, the
noise rises with the velocity, i.e. the faster the process, the less robust the process. At $v_0 > 19\ \mu\text{m/s}$, the inversion breaks down. Unlike the linear case, the transfer completeness $P$ does not tend to zero but to the negative value $P \approx -0.7$. This means that $z(0)$ and $z(T)$ have the same sign, i.e. the process results only in a modest population transfer, keeping the initial inequality $N_L > N_R$ at $t=T$.

In Figure 5, the similar analysis is done for the softer (more adiabatic) velocity profile $v_s(t)$. The results are very similar to those in Fig. 4. The only but important difference is that, in the repulsive BEC, the inversion at $v_0 \leq 20\ \mu\text{m/s}$ is accompanied by much less noise as compared to the previous $v_c(t)$ case (see plot d)). So, as might be expected, the softer (and thus more adiabatic) velocity profile $v_s(t)$ provides a much better inversion than the sharp profile $v_c(t)$.

The physical sense of the critical velocity $v_{crit} \approx (19-20)\ \mu\text{m/s}$ which marks the break of inversion for both $v_c(t)$ and $v_s(t)$ regimes should be clarified. Following our analysis, $v_{crit}$ does not correspond to the destruction of adiabaticity (indeed we have about the same $v_{crit}$ for less and more adiabatic profiles $v_c(t)$ and $v_s(t)$), but is rather determined by the transfer capacity defined as the multiplicative effect of the barrier penetrability $w$ and transfer duration $T$. Just these two values suffice to control the number of atoms to be transferred. Time $T$ can be enough ($v_0 < v_{crit}$) or not ($v_0 > v_{crit}$) for the complete inversion. For the repulsive BEC, the barrier penetrability $w$ is high and so the full inversion can be fast which explains the high $v_{crit}$ and wide NLPI plateau in Figs. 4 b) and 5 b). In the ideal BEC, the penetrability $w$ is much weaker and thus longer times (lower velocities) are necessary for the inversion. Altogether, we see a strong support of the inversion by the repulsive interaction. The nonlinearity does not destroy but instead greatly favours the inversion, making it much faster.

These findings are in accordance with our previous results for the complete transport of BEC from the left to the right well, obtained within the simplified model employing the two-mode approximation \cite{8}. In that study, the appearance of a wide velocity plateau due to the repulsive interaction was also observed. Note that velocity of the process has a lower limit (e.g. caused by the finite lifetime of BEC, which is commonly a few seconds).

**IV. SUMMARY**

The complete population inversion of the repulsive BEC in a double-well trap was investigated within the time-dependent three-dimensional Gross-Pitaevskii equation, following parameters of experiments of the Heidelberg group \cite{13,14}. The calculations are performed beyond usual approximations (two-mode, etc) in the description of tunneling and transport dynamics. The inversion is driven by a time-dependent barrier shift performed with different velocity regimes. As might be expected, a soft velocity profile $v(t)$ gives a more robust inversion than the sharp one.

The most remarkable result is a significant support of the complete inversion by the repulsive interaction between BEC atoms. Due to the interaction (and related nonlinearity of the problem), the inversion can be produced in a wide velocity interval. Moreover, the process can be three orders of magnitude (!) faster than in the ideal BEC. Thus the transfer can be done far beyond the adiabatic requirements. These results are in accordance with our previous findings obtained within the two-mode approximation approach \cite{8}. The interaction effect is mainly reduced to the rise of chemical potential. Hence it should depend on the barrier form, being strong for barriers whose penetrability increases with the excitation energy and suppressed for barriers with energy-independent penetrability.

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