Tunneling and transport dynamics of trapped Bose-Einstein condensates

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Abstract. We present particular examples of tunneling and transport dynamics of Bose-Einstein condensate (BEC) in a two-well trap: Josephson oscillations (JO), macroscopic quantum self-trapping (MQST) and complete adiabatic transport. Being quite general, these dynamical regimes have close analogies with Josephson junctions in superconductors and transport problems in nanosystems. The calculations are performed within the time-dependent mean-field prescription within (transport) and beyond (JO and MQST) two-mode approximation. For the transport a universal adiabatic population transfer scheme is proposed, allowing a robust and complete transport even under strong nonlinear effects.

1. Introduction

Nowadays the trapped Bose-Einstein condensate (BEC) is widely recognized as a source of new fascinating physics and remarkable cross-over with other areas, see e.g. monographs [1, 2] and recent reviews [3, 4, 5, 6]. In this broad field, the dynamics of weakly bound BECs in two-well systems is now of a keen interest. Its fundamental features and numerous links to other subjects (Josephson junctions [3, 7, 8, 9, 10, 11], optical lattices [3, 4, 6], transport problems [12, 13, 14, 15, 16, 17], topological states [18, 19] etc.) are indeed of a general interest.

In this paper we present some particular examples of tunneling and transport dynamics of BEC in a two-well trap, which might be interesting not only for BEC community but also for experts from various branches of nanophysics. First, Josephson oscillations (JO) of BEC are considered and compared with those in superconductor Josephson junctions (SIJ) [9]. Then the macroscopic quantum self-trapping (MQST) is exhibited [7, 8]. This effect takes place in Bose Josephson junction (BJJ) but not in the SIJ [9]. Finally, the adiabatic transport of BEC between the trap wells is considered. Usually such transport heavily suffers from the nonlinearity caused by the interaction between BEC atoms [20, 21]. To overcome this trouble, we propose some universal adiabatic transport protocols [16, 17] which work even at strong nonlinearity. The protocols are developed on the basis of Landau-Zener [22] and Rosen-Zener [23] schemes.

The calculations were performed with the Gross-Pitaevski equation [24]. It was directly solved in 3D coordinate grid space for JO and MQST and treated in the two-mode approximation [7, 8, 9] for more complicated transport problem.
2. Formalism

The calculations were performed in the mean-field approximation by solving the time-dependent Gross-Pitaevski equation [24]

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

where \( \Psi(\vec{r}, t) \) is the classical order parameter of the system, \( V(\vec{r}, t) \) is the double-well trap potential, \( g_0 = 4\pi\hbar^2a_s/m \) is the parameter of interaction between BEC atoms, \( a_s \) is the s-scattering length and \( m \) is the atomic mass.

For JO and MQST, the static confinement \( V(\vec{r}) \) is used and Eq. (1) is directly solved by implementation of Hartree-Fock (HF) static and time-dependent algorithms for 3-dimensional systems [25]. Only the lowest level occupied by BEC is involved into HF procedure. Note, that in most of the previous JO and MQST studies [7, 8, 9, 10] performed within the two-mode approximation (TMA), the energy of the ground state \( E_1 \) and corresponding barrier penetrability \( K \) were approximated by constants independent on the number of BEC atoms \( N \) and interaction \( g_0 \). In the present approach, the energy and penetrability are calculated self-consistently and depend on \( N \) and \( g_0 \). Note that the difference between TMA and HF results at a strong interaction can be essential [26].

For more complicated transport problem with the time-dependent confinement in a double-well trap, we however are enforced to use the TMA [7, 8, 9]:

\[ \Psi(\vec{r}, t) = \sqrt{N}(\psi_1(t)\Phi_1(\vec{r}) + \psi_2(t)\Phi_2(\vec{r})) \] (2)

where \( \Phi_k(\vec{r}) \) is the static ground state solution of (1) for the isolated k-th well \( (k = 1, 2) \) and

\[ \psi_k(t) = \sqrt{N_k(t)}e^{i\phi_k(t)} \] (3)

is the expansion amplitude expressed via the normalized population \( N_k(t) \) and phase \( \phi_k(t) \). The total number of atoms \( N \) is fixed: \( \int d\vec{r} |\Psi(\vec{r}, t)|^2/N = N_1(t) + N_2(t) = 1 \).

Substituting (2)-(3) to (1) and integrating out the spatial distributions \( \Phi_k(\vec{r}) \) we get the system of equations for the populations \( N_k(t) \) and phases \( \phi_k(t) \) [8]:

\[ N_k = -2\Omega(t)\sqrt{N_jN_k} \sin(\phi_j - \phi_k) \] (4)

\[ \dot{\phi}_k = -[E_k(t) + UN_k] + \Omega(t)\sqrt{N_j/N_k} \cos(\phi_j - \phi_k) \] (5)

with \( j \neq k \). Here

\[ \Omega(t) = -\frac{1}{\hbar} \int d\vec{r} \left[ \frac{\hbar^2}{2m} \nabla \Phi_1^* \cdot \nabla \Phi_2 + \Phi_2^* V(t) \Phi_1 \right] \] (6)

is the coupling between BEC fractions (= barrier penetrability),

\[ E_k(t) = \frac{1}{\hbar} \int d\vec{r} \left[ \frac{\hbar^2}{2m} |\nabla \Phi_k|^2 + \Phi_k^* V(t) \Phi_k \right] \] (7)

is the depth of the k-th well and

\[ U_k = \frac{g_0}{2\hbar} \int d\vec{r} |\Phi_k|^4 \] (8)

labels the interaction between BEC atoms in the same well (here \( U_1 = U_2 = U \)). The values \( \Omega(t), E_k(t) \) and \( U \) have the dimension of frequency.
Considering $N_k$ and $-\phi_k$ as conjugate variables and using the linear canonical transformation [21], $z = N_1 - N_2$ and $\theta = \frac{1}{2}(\phi_2 - \phi_1)$, one may extract the integral of motion $N$ and the total phase, thus reducing the problem to finding the population imbalance $z$ and phase difference $\theta$:

\[
\dot{z} = -\bar{\Omega}(t)\sqrt{1 - z^2}\sin 2\theta \\
\dot{\theta} = \frac{1}{2}[\Delta(t) + \Lambda z + \bar{\Omega}(t)\frac{z}{\sqrt{1 - z^2}}\cos 2\theta]
\]

where

\[
\bar{\Omega}(t) = \frac{\Omega(t)}{K}, \quad \bar{E}_k(t) = \frac{E_k(t)}{2K}, \quad \Delta(t) = \bar{E}_1(t) - \bar{E}_2(t), \quad \Lambda = \frac{UN}{2K}
\]

are the dimensionless coupling, well depths, detuning and interaction, scaled by the coupling amplitude $K$. The time in (9)-(10) is also scaled by $2K$ and so is dimensionless. The key parameter $\Lambda$ representing the interaction-coupling ratio is decisive in the tunneling dynamics. In JO and MQST problems, we use the static symmetric trap with $\bar{\Omega}(t)=1$ and $\Delta(t)=0$ while for transport we deal with time-dependent $\bar{\Omega}(t)$ and $\Delta(t)$.

Eqs. (9)-(10) can be also derived as canonical equations for the conjugate variables $z$ and $\theta$ and the classical Hamiltonian

\[
H_{cl} = \frac{1}{2}[\Delta(t)z + \Lambda z^2 - \bar{\Omega}(t)\sqrt{1 - z^2}\cos 2\theta].
\]

3. JO and MQST

Josephson Oscillations and Macroscopic Quantum Self-Trapping represent the main regimes of BEC tunneling dynamics in a double-well trap. A weak coupling of BEC fractions through the barrier is assumed. Here we consider the static trap $V(x)$ of symmetric configuration ($\Delta=0$). The static barrier penetrability is $\bar{\Omega} = K$, i.e. $\bar{\Omega}=1$. JO are explored for the ideal BEC (no interaction, $U = 0$) while MQST is discussed for the repulsive interaction between BEC atoms ($U > 0$). The calculations are performed for $N=100$ BEC atoms. The initial state is computed with $\sim 15000$ static iterations.

Figure 1a) demonstrates the double-well confinement $V(x)$, the energy spectrum $E_n$ and the initial density $\rho(x)$ of the ideal BEC. Since the isolated wells are described by equal oscillator potentials with the frequency $\omega_0$ and oscillator length $a_0$, it is convenient to give the values in Fig. 1 in natural units of length $a_0$, frequency $\omega_0$ and time $\omega_0^{-1}$. The h.o. levels below the barrier are known to be split into two sublevels [27]. Magnitude of the splitting $\Delta E$ is determined by the barrier penetrability $K$ at the level energy, and related to the JO frequency. In our case of weak coupling, the splitting of the lowest h.o. level, $\Delta E = E_2 - E_1 \sim 0.01\omega_0$, is very small and not visible in the figure. Actually the sublevels $E_n$, $n=1-5$, look in Fig. 1a as 2 levels.

In Fig. 1, the time evolution starts from the non-stationary state ($N_1 = 1, N_2 = 0, z = N_1 - N_2 = 1$) and the tunneling gives the non-stop Josephson or Rabi oscillations, see Fig. 1b. The non-stop regime arises for the energy conservation reason. If the system is isolated and BEC energy (12) is conserved, then the non-stationary state with initial $z(0) = 1, \theta(0) = 0$ is unable to relax into the stationary state ($N_1 = N_2 = 0.5, z = 0$) with another energy, hence endurant oscillations. For ideal BEC in the symmetric trap, the JO frequency is $\omega_{BJJ} = 2K$ [8], i.e. is determined by the barrier penetrability at $E_1 \approx \bar{E}_2$. Fig. 1b demonstrates JO for two well separations, $d = 5$ and $6a_0$. For $d = 6a_0$, the barrier at $E_1 \approx \bar{E}_2$ is wider and so $\omega_{BJJ}$ is smaller.

It is instructive to compare the dynamics in Bose and superconductor Josephson junctions, i.e. BJJ vs SJJ [3, 28]. There are obviously some similarities: in both cases we deal with tunneling between left and right states and get the alternating current (ac). At the same time, there are significant differences. First, in the above example, BJJ gives ac for $\Delta=0$, i.e. without
Figure 1. Mean-field characteristics (left) and Josephson oscillations (right) of the ideal BEC in a double-well trap with well separations $d = 5a_0$ (upper) and $d = 6a_0$ (bottom). The left plots exhibit confinement field $V(x)$ (solid curve), lowest 5 energy levels $E_n$ (solid horizontal lines) and initial BEC density $\rho(x)$ (dash curve). The right plots give populations $N_1(t)$ (solid curve) and $N_2(t)$ (dotted curve) of the fist and second wells, respectively.

Figure 2. The population imbalance $z(t)$ in quasiharmonic (a), anharmonic (b), and MQST (c) tunneling regimes for scattering lengths $a_s$ as indicated. The well separation is $d = 5a_0 = 6.1\mu m$ for all the plots.

the potential difference. Instead, SJJ has ac only at nonzero applied voltage $eV_s = E_1 - E_2$ and gives the direct current (dc) for $V_s=0$, see e.g. [30, 31]. Second, the BJJ ac frequency $\omega_{BJJ} = 2K$ is determined by the barrier penetrability, i.e. by the system configuration. In contrast, the SJJ ac frequency $\omega_{SJJ} = 2eV_s/\hbar$ is determined by the applied voltage and does not depend on the system configuration.

Actually, the difference between BJJ and SJJ oscillations can be put away by considering Eqs. (9)-(10) in the limit $K \ll \Delta$ instead of $K \gg \Delta$ used above [8]. Then the BJJ frequency is reduced to $\omega_{BJJ} = E_1 - E_2$ in accordance to the SJJ case. Note that the limit $K \ll \Delta$ is typical for SJJ while BJJ can deal with both $K \ll \Delta$ and $K \gg \Delta$ options. The more detailed comparison of BJJ and SJJ ac can be found in the recent study [32].
Another physical situation arises in BJJ if the interaction between BEC atoms comes to play. This is demonstrated in Fig. 2 for different values of the repulsive interaction characterized by the scattering length $a_s$. Here, to give an idea of the typical scales, the values $a_s$, $d$ and time $t$ are given in standard units. Fig. 2 shows that increasing the interaction leads to anharmonicity of oscillations (plot b)) and finally to the self-trapping regime (MQST) with the time average $< z > = 0.5$ (plot c)). In the later, BEC oscillates not around the stationary state with $< z > = 0$ like in plots a)-b) but around the non-stationary initial population with nonzero $< z >$. Thus the main BEC part is permanently trapped in the left well. The JO and MQST for the repulsive BEC were observed in experiment [11]. MQST takes place at sufficiently strong interaction or, at fixed $\Lambda > 0$, at a large initial population imbalance $|z(0)|$[7, 8, 9]. Though the self-trapping or self-locking is a general phenomenon existing in many physical systems [29], it occurs in the BJJ but not in SJJ. In BJJ the effect depends on the initial phase difference, e.g. is quite different for $\theta(0)=0$ (present case) and $\pi$ [9].

4. Adiabatic transport
The transport of BEC in a two-well trap assumes that BEC, being initially in one of the wells, is then completely transferred in a controllable way to the target well and kept there. In principle such a transport can be produced by many methods, see discussion in [16]. However, most of these methods do not work even at modest nonlinearity. In this connection, we have recently proposed a novel adiabatic transport protocol [16] based on the generalization of Landau-Zener [22] and Rosen-Zener [23] schemes. The protocol is robust to a strong nonlinearity and can be applied to both repulsive and attractive BEC.

Figure 3. a) The double-well trap with time dependent ground state energies $E_1(t)$ and $E_2(t)$, detuning $\Delta(t)$, and coupling (barrier penetrability) $\Omega(t)$. The BEC is initially placed at the first (left) well as indicated by the bold dot. Then it is transferred to the 2nd (right) well as indicated by the bold arrow. b) Time evolution of the coupling $\Omega(t)$ and detuning $\Omega(t)$.

The protocol scheme is illustrated in Fig. 3. As seen from the plot b), the transport is driven by simultaneous varying the well depths and coupling (barrier penetrability). At the initial time, the trap is asymmetric ($E_1 < E_2$) and the barrier is actually impenetrable ($\Omega=0$). Then the well depths evolve to get the opposite asymmetry $E_1 > E_2$. Simultaneously the barrier narrows and becomes penetrable, providing the coupling between BEC fractions in the neighboring wells. Just that time the BEC transfer occurs. Finally, the well evolution stops, the barrier becomes again impenetrable ($\Omega=0$) and the transport is over. In the present study, the evolution of wells and coupling are linear and Gaussian, respectively,

$$\Delta(t) = E_1(t) - E_2(t) = \alpha t, \quad \Omega(t) = \exp\left\{-\frac{(\tilde{t} - t)^2}{2\Gamma^2}\right\} , (13)$$

where $\alpha$ is the detuning rate and $\tilde{t}$ and $\Gamma$ are the centroid and width parameters. Obviously, this protocol is a generalization of the Landau-Zener (linear change of $\Delta(t)$ and constant $\Omega$)
and Rosen-Zener (constant $\Delta$ and pulse $\tilde{\Omega}(t)$) schemes [22, 23]. In the experimental setup, the drives (13) can be routinely produced by imposing an additional modulation field and changing the separation between the wells.

Results of the calculations in the two-mode approximation are given in Figs. 4 and 5 [16]. Fig. 4 shows the final transport result, the population $P = N_2(t \to \infty)$ of the 2nd well, at various detuning rate $\alpha$ and nonlinearity $\Lambda$. It is seen that for ideal BEC ($\Lambda=0$) the complete adiabatic transport is possible only at very slow detuning rate, $\alpha \to 0$. The repulsion interaction ($\Lambda > 0$) creates a plateau in $P(\alpha)$ dependence where the transport is robust and complete. The stronger the BEC interaction, the wider the plateau. Hence in the present protocol, the interaction and related nonlinearity even favor the transport by enlarging the active $\alpha$ interval. At larger rates, say $\alpha > 7$ for $\Lambda = 10$, the process becomes too fast and the adiabatic transfer vanishes. Note a narrow $P=0$ window at small rates $\alpha$ in the interacting BEC. A sharp rise of the transfer at the right window boundary can be used for switching the transport by a small tuning of $\alpha$.

The robustness of the transport of the repulsive BEC is justified in Fig. 5a for the particular case of $\Lambda = 4$ and $\alpha = 3$. It is seen that indeed the population $N_1 = 1, N_2 = 0$ at early time is transformed to the population $N_1 = 0, N_2 = 1$ at late time.

An opposite situation takes place for the attractive BEC with $\Lambda < 0$. Figs. 4b and 5b show that the complete transport fails, and the stronger the nonlinearity, the more the failure. There is no any plateau, the final population $P$ of the interacting BEC is small, and main part of BEC still remains in the initial well.
However, due to the symmetry of the problem (9)-(10)

\[
\Lambda \rightarrow -\Lambda, \quad \alpha \rightarrow -\alpha, \quad \theta \rightarrow -\theta + \frac{\pi}{2}
\]

or

\[
\alpha \rightarrow -\alpha, \quad z \rightarrow -z, \quad \theta \rightarrow -\theta,
\]

the transport protocol can be recast and provide again the robust and complete transfer [16].

Actually, (14) relates the transport protocols for repulsive and attractive BEC in one direction while (15) connects the transport in opposite directions (with corresponding interchange of the initial conditions). Specifically the left-right transport \(|1\rangle \rightarrow |2\rangle\) with the initial populations \(N_1 = 1, N_2 = 0\) should use \(\alpha > 0\) for \(\Lambda > 0\) and \(\alpha < 0\) for \(\Lambda < 0\) where \(\alpha < 0\) means that the initially occupied left well should be higher than the right one. Instead the right-left transport \(|1\rangle \leftarrow |2\rangle\) with the initial populations \(N_1 = 0, N_2 = 1\) should use \(\alpha < 0\) for \(\Lambda > 0\) and \(\alpha > 0\) for \(\Lambda < 0\).

The above discussion demonstrates a universal character of our transport protocol. It can be also used for other scenarios, e.g. for the transfer of BEC between its two components in a single-well trap. In this case BEC contains atoms in two different hyperfine levels, thus forming two components. The time-dependent laser pulse \(\Omega(t)\) couples the components and initiate the population transfer. The evolution of the detuning is produced by the additional Stark pulse. Such scheme is already used in the Stark Chirped Rapid Adiabatic Passage (SCRAP) method [33] for the population transfer in atoms and simple molecules.

5. Conclusions

The examples of tunneling dynamics in a double well system (Josephson oscillations, macroscopic quantum self-trapping and adiabatic transport) were illustrated and discussed. Being very general, these kinds of dynamics can be met in various systems including those of nano size. In particular, they take place in two-level systems with the laser coupling where they are called as Rabi oscillations, self-locking and adiabatic population transfer. Comparison of these dynamical regimes in different physical situations can be extremely useful for better understanding the basic physics behind. In this connection, the trapped Bose-Einstein condensate which allows an effective control on the process parameters and thus accesses various physical scenarios can serve as a unique laboratory of fascinating physics with numerous crossover with other topics.

Acknowledgments

The work was supported by the grants 08-0200118 (RFBR, Russia), 684 (Université Paul Sabatier, Toulouse, France, 2008), 202/06/0363 and MSM 0021620859 (Ministry of education of the Czech Republic), and Votruba - Blokhintsev (Czech Republic - BLTP JINR). We are grateful to A Yu Cherny and V I Yukalov for help and useful discussions.

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