Probing two-particle exchange processes in two-mode Bose-Einstein condensates

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We study the fidelity decay and its freeze for an initial coherent state of two-mode Bose-Einstein condensates in the Fock regime considering a Bose-Hubbard model that includes two-particle tunneling terms. By using linear-response theory we find scaling properties of the fidelity as a function of the particle number that prove the existence of two-particle mode-exchange when a non-degeneracy condition is fulfilled. Tuning the energy difference of the two modes serves to distinguish the presence of two-particle mode-exchange terms through the appearance of certain singularities. Numerical results confirm our findings. Experimental verification of our findings could improve cold atom interferometry.

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The Bose-Hubbard model became a workhorse to describe interactions of ultracold bosonic gases trapped by neighboring potentials after its striking success with the Mott insulator-superfluid transition. Its most simple physical realization, when only two bosonic states can be occupied, is experimentally realized by trapping the condensate in a double-well potential. This system is interesting because it is the simplest scheme for atom interferometry. In addition to interference phenomena, it also exhibits quantum tunneling and self trapping effects such as Josephson oscillations. It has even been used to produce and study many-particle entanglement and dynamically generate spin-squeezed states. Alternative methods to optical lattices have been demonstrated by splitting a single-component Bose-Einstein condensate (BEC) on atom chips either with pure DC magnetic fields or by dressing static fields with RF potentials as proposed in. Understanding the effects originated on inter-atomic collisions has already been exploited to overpass the classical limit in atom interferometers, for example. Here we employ an extended Bose-Hubbard Hamiltonian to increase the possibilities in this direction.

Several interchange terms arise in the Bose-Hubbard model in a double-well potential where only the lowest level in each well is populated and the corresponding wave functions have a small overlap. In particular, two terms accounting for two-particle mode-exchange processes appear in the derivation of the Hamiltonian. These terms are often neglected assuming that two-particle processes are rare for diluted ultracold gases. Yet, Ref. points out that there is a better agreement with the experimental results when these processes are included. In this paper we probe the relevance of these terms by studying dynamical properties linked with two-particle tunneling processes. We consider the dynamical stability of the quantum evolution under small system perturbations for the two-mode Bose-Hubbard model using the fidelity or Loschmidt echo, whose decay has been studied for different parameter ranges or types of perturbations in the Bose-Hubbard model.

Prosen and Žnidarič noticed that fidelity stops decaying, staying essentially constant (modulo some oscillations) for relatively long times whenever the time-averaged expectation value of the perturbation vanishes. This phenomenon is called fidelity freeze. It was later shown that symmetries can also induce this behavior if the diagonal matrix elements of the perturbation vanish, e.g. when the perturbation is not invariant under the time-reversal symmetry. Note that the freeze of fidelity was actually observed in simulations for bosonic and fermionic many-body systems, but it was attributed to the non-linearities introduced by the interactions between the particles. Our purpose is to draw attention to this phenomenon, and exploit it, within the context of the Bose-Hubbard model. We show analytically and numerically that the scaling properties of the fidelity freeze $F_{Fr}$ associated to an initial macroscopic trial state display a transition in terms of the number of particles if the interaction includes two-particle mode-exchange terms. In addition, when certain degeneracy condition is fulfilled by tuning the energy difference of the two wells, the fidelity freeze tends abruptly to zero. This yields insight into many-body tunneling processes and provides a method to calibrate the system to enhance the fidelity freeze.

The fidelity amplitude is the overlap of the time-evolution of an initial state under a reference interaction $\hat{H}_0$ with the evolution of the same initial state under a slightly different Hamiltonian $\hat{H} = \hat{H}_0 + \lambda \hat{V}$:

$$ f(t) = \langle \Psi_0 | \hat{U}_0(-t) \hat{U}_\lambda(t) | \Psi_0 \rangle. $$

Here, $| \Psi_0 \rangle$ is the initial state under consideration, $\hat{U}_0(t) = T \exp[-i \hat{H}_0 t / \hbar]$ is the (time-ordered) unitary
time-evolution associated to the reference Hamiltonian, $\hat{U}_\lambda(t)$ is the corresponding time-evolution of the perturbed Hamiltonian, and the perturbation strength is denoted by $\lambda$. The modulus squared of the fidelity amplitude, $F(t) = |f(t)|^2$, is the fidelity or Loschmidt echo \cite{21, 22}. Clearly, $F(t)$ is a measure of the sensitivity of the time evolution of $|\Psi_0\rangle$ to system perturbations. Another interpretation is that of an echo: $|\Psi_0\rangle$ evolves under $H_0$ up to time $t$, then the system is suddenly reversed with respect to time, and then evolves under the action of $\hat{H}$; the Loschmidt echo compares the whole evolution with the initial state, thus quantifying the degree of irreversibility of the system. The operator $M_\lambda(t) = \hat{U}_\lambda(-t)\hat{U}_0(t)$ is referred as the echo operator.

We consider the generalized Bose-Hubbard model $\hat{H}_{BH} = H_0 + V$ defined by

$$\hat{H}_0 = \epsilon_1 \hat{n}_1 + \epsilon_2 \hat{n}_2 + \frac{U}{2} \left[\hat{n}_1(\hat{n}_1 - 1) + \hat{n}_2(\hat{n}_2 - 1)\right], \quad (2)$$

$$\hat{V} = -J_1 (\hat{b}_1^\dagger \hat{b}_2 + \hat{b}_2^\dagger \hat{b}_1) - \frac{J_2}{2} \left[ (\hat{b}_1)^2 \hat{b}_2^2 + (\hat{b}_2)^2 \hat{b}_1^2 \right]. \quad (3)$$

As usual, $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ ($i = 1, 2$) is the particle number operator of the $i$-th mode, with $\hat{b}_i^\dagger$ and $\hat{b}_i$ the corresponding bosonic creation and annihilation operators, respectively. The single-particle energies of each mode are denoted by $\epsilon_i$, $U$ is the two-particle on-site interaction, $J_1$ is the energy of the usual (one-particle) Josephson tunneling or mode-exchange term, and $J_2$ is the energy associated to two-particle tunneling processes that we probe here. The total number of particles $n = n_1 + n_2$ is a conserved quantity; fixing $n$, the Hilbert-space dimension is simply $n + 1$. The Hamiltonian $\hat{H}_{BH}$ defined through Eqs. (2) and (3) is a generalization of the usual two-mode approximation used to describe the bosonic Josephson junction \cite{31, 32}.

We are interested in the case where $U \gg J_1 > J_2$, the so-called the Fock regime. Then, a convenient basis is the occupation number basis, or Fock basis, defined by $|\mu_1, \mu_2\rangle = \langle \mu_1 | \mu_2 \rangle^{-1/2} (\hat{b}_1)^{\mu_1} (\hat{b}_2)^{\mu_2} |0\rangle$, where $|0\rangle$ is the vacuum state; since $n = \mu_1 + \mu_2$ is conserved, we shall use the short-hand notation $|\mu\rangle \equiv |\mu_1, \mu_2\rangle$. By definition, $\hat{H}_0$ is diagonal in the Fock basis and $\hat{V}$ has vanishing diagonal matrix elements. Considering $\hat{H}_0$ as the reference interaction and $\hat{V}$ as the perturbation or residual interaction, the conditions to observe the fidelity freeze are fulfilled \cite{28}. The unperturbed spectrum is simply given by $E_\mu = E_0 + \epsilon_1 + \epsilon_2 - U n + \mu^2 U$ with $E_0 = \epsilon_2 n + U n (n - 1)/2$. As it is often done we use the Heisenberg time $t_H = 2\pi \hbar/\overline{d}$ as the unit of time, where $\overline{d}$ is the average level spacing of the unperturbed Hamiltonian $\hat{H}_0$.

We compute the fidelity decay by noting that $M_\lambda(t)$ is the time-evolution propagator associated with the time-dependent Hamiltonian $\hat{V}_\lambda(t) = \hat{U}_\lambda(t)\hat{V}\hat{U}_0(t)$ in the interaction picture \cite{31}. We use Dyson’s series on the perturbation parameters $J_r$ ($r = 1, 2$) truncated to the second order \cite{31, 32}. This approach is called linear response theory.

We write the fidelity amplitude as $f(t) = 1 + f_1 + f_2 + O(J_r^2)$, where the first- and second-order corrections (in both $J_1$ and $J_2$) explicitly read

$$f_1 = \sum_{\mu, \nu} A^*_{\mu} A_{\nu} V^{(r)}_{\mu, \nu} \langle I_1(t) | \Omega_{\mu, \nu}, \rangle, \quad (4)$$

$$f_2 = \sum_{r, s, \mu, \nu, \rho} A^*_{\mu} A_{\nu} V^{(r)}_{\mu, \rho} V^{(s)}_{\rho, \nu} \langle I_2(t) | \Omega_{\mu, \rho}, \Omega_{\rho, \nu}, \rangle. \quad (5)$$

Here, the matrix elements of the perturbation in the interaction picture are $\langle \mu | \hat{V}_\lambda(t) | \nu \rangle = \sum_{\rho} V^{(r)}_{\mu, \rho} \exp[i\Omega_{\mu, \rho} t]$ and $\hat{H}_{\mu, \nu} = E_\mu - E_\nu$, and $A_{\mu}$ are the expansion coefficients of the initial state in the Fock basis. In Eqs. (4) and (5), greek letters represent the basis states and $r, s$ stand for the one- or two-particle tunneling terms of $\hat{H}_{BH}$. These matrix elements read

$$V^{(r)}_{\mu, \nu} = f_r (g^{(r)}_{\mu, \nu} \delta_{\mu, \nu} - g^{(r)}_{\nu, \mu} \delta_{\mu, \nu}) \left[ \langle \mu | \hat{V}_\lambda(t) | \nu \rangle \langle \nu | \hat{V}_\lambda(t) | \mu \rangle \right]. \quad (6)$$

The time dependence of Eqs. (4) and (5) appears in the (time-ordered) integrals $I_p[t; \Omega_1, \ldots, \Omega_p]$, where $p$ stands for the order in the Dyson’s series. These integrals can be expressed recursively as

$$I_{p+1}[t; \Omega_1, \ldots, \Omega_{p+1}] = -\frac{i}{\hbar} \int_0^t dt_1 \exp[i\Omega_1 t_1] I_p[t_1; \Omega_2, \ldots, \Omega_{p+1}], \quad (8)$$

where $I_0[t] = 1$ defines the initial value of the recursion. These integrals produce terms that oscillate in time as long as the frequencies $\Omega_{\mu, \nu}$ appearing in the exponentials do not vanish, i.e. when the unperturbed spectrum is non-degenerate. Yet, certain frequency combinations may vanish and yield secular terms which grow at least linearly in time. We assume that the unperturbed spectrum is non-degenerate, which can be assured by choosing properly the energy difference of the two modes $\Delta \epsilon = \epsilon_2 - \epsilon_1$. Then, without the secular contributions, to second-order the fidelity displays quasi-periodic oscillations in time; this is the freeze of the fidelity. The freeze of the fidelity lasts as long as the second-order approximation is valid; eventually, higher-order contributions dominate the evolution and secular terms appear that destroy the freeze of the fidelity.

Equation (7) is valid for any initial state. We consider as the initial state a normalized macroscopic trial state of the form \cite{30}

$$|\Psi_0\rangle = (\alpha \hat{b}_1^\dagger + \beta \hat{b}_2^\dagger)^n |0\rangle = \sum_{\mu} \langle n | \mu \rangle 1/2 \langle \mu | \hat{b}_1^\dagger \hat{b}_2^\dagger \rangle \alpha^{\mu} \beta^{n-\mu} e^{i(n-\mu)\phi} |\mu\rangle. \quad (9)$$
This initial state is coherent \(|\Phi\rangle\), with \(\alpha = (n_1/n)^{1/2}\) and \(\beta = (n_2/n)^{1/2}\), it corresponds to the mean-field state having \(n_1\) particles in the first mode and \(n_2 = n - n_1\) in the second one.

Inserting Eqs. (9) and (10) in (8) and (9), we obtain

\[
\begin{align*}
F_{r,t} &= 1 + 2 \sum_{r,s} |A_{r,s}^+| A_{r,s}^- |G_{r}^{(+s)}(\phi) - G_{s}^{(-r)}(\phi)|^2 + 2 \sum_{r,s} |A_{r,s}^+| A_{r,s}^- |G_{r}^{(+s)}(\phi) - G_{s}^{(-r)}(\phi)|^2 \\
&= 1 + 2 \sum_{r,s} |A_{r,s}^+| A_{r,s}^- |G_{r}^{(+s)}(\phi) - G_{s}^{(-r)}(\phi)|^2 + 2 \sum_{r,s} |A_{r,s}^+| A_{r,s}^- |G_{r}^{(+s)}(\phi) - G_{s}^{(-r)}(\phi)|^2
\end{align*}
\]

The coefficients \(G^{(r)}_{\mu} = g^{(r)}_{\mu,n-\rho,r+s}\) and \(G^{(s)}_{\mu} = g^{(s)}_{\mu,n-\rho,s-r}\) are introduced to have a more compact expression. The signs of \(r\) and \(s\) are independent and correspond to the distinct possibilities imposed by the Kronecker deltas that appear in Eqs. (10) and (11). Equation (15) is a central result of this paper.

In Fig. 1 we show an example of the decay of fidelity for a coherent state with \(n_1 = n_2 = n/2\) and \(\phi = \pi/4\) obtained numerically. The figure illustrates the oscillations during the freeze of the fidelity, the eventual decay, and the value obtained from Eq. (15) for the freeze of the fidelity (horizontal green line). Time is measured in Heisenberg-time units \(t_H\). The parameters of the model are \(U = 1, J_1 = 10^{-6}, J_2 = 10^{-8}, \epsilon_1 = 0.76, \epsilon_2 = 0.93\) and \(n = 128\); the values of \(\epsilon_i\) assure the non-degeneracy of the spectrum of \(H_0\). In the inset we display the result considering the second-order expansion \(\bar{\epsilon}\); the value of the fidelity freeze clearly corresponds to an average over the quasi-periodic oscillations that take place during the freeze.

We address now the scaling of \(F_{r,t}\) in terms of the number of particles. An estimate of the scaling properties is obtained considering the maximum contribution of the \(n\)-dependent terms in Eq. (15). This follows from a Fock state that we write as \(\mu = \lambda n\), and then use Stirling’s formula for large \(n\). It can be shown that \(A_{\mu}^\dag A_{\mu}^\dagger \sim n^{1/2}\) and \(G^{(s)}_{\mu} \sim n^s\) for \(\lambda = \alpha^2\). The scaling laws of the time-independent contributions thus read \(\Re(f_{1,2}) \sim n^{r-1/2}\) and \(\Re(|f_1|^2) \sim n^{2r-1}\). Hence, the dominating contribution for the fidelity freeze scales as

\[1 - F_{r,t} \sim J_r^2 n^{2r-1/2}.\] (16)

This result predicts a different scaling for each of the tunneling terms \(J_1\) and \(J_2\). Thus, \(F_{r,t}\) exhibits a transition from a behavior dominated by \(J_1\) to a regime where the coefficient \(J_2\) has a stronger influence in terms of \(n\),
around $n \sim J_1/J_2$. Figure 2 is the numerical confirmation of this statement. The data points were obtained numerically from time series (cf. Fig. 1), using the maxima of the quasi-periodic oscillations of $1 - F(t)$ during the freeze; these values underestimate the theoretical expectation for $F_{Fr}$. Fitting the data to straight-lines when either $J_2$ or $J_1$ are absent yields the slopes 1.52 and 3.54, respectively. These values are in excellent agreement with the 3/2 and 7/2 predicted by Eq. (16), thus showing that the scaling properties of the fidelity freeze in terms of $n$ probe the presence of two-particle tunneling processes. Note that Eq. (16) holds for $k$-particle tunneling perturbations of the form $[\langle \hat{b}_1 \rangle^k \hat{b}_2 + \langle \hat{b}_2 \rangle^k \hat{b}_1]/k!$.

An important assumption that we made in the derivation of Eqs. (15) and (16) is that the spectrum of $\hat{H}_0$ is non-degenerate, which can be fulfilled by tuning $\Delta \epsilon$, the energy difference of the two modes. As we approach the degeneracy, the appearance of secular terms makes Eq. (15) no longer valid. This can be exploited to probe the relevance of two-mode exchange processes.

To clarify this idea we consider the Fock state $\mu_0 = [(n + \Delta \epsilon/U)/2]$ whose energy is the minimum of the spectrum of $\hat{H}_0$, where $|x|$ is the round-to-nearest integer function. Assuming that $n$ is even for concreteness, it can be shown that $\Delta \epsilon/U = 0$ implies that $E_{\mu_0-1} = E_{\mu_0+1}$, meaning that the Fock states $\mu_0 - 1$ and $\mu_0 + 1$ are degenerate; these states are coupled by a two-mode tunneling term. The same holds for $\Delta \epsilon/U = 2$, though the actual value of $\mu_0$ has changed. For $\Delta \epsilon/U = 1$ we have

$E_{\mu_0} = E_{\mu_0+1}$, i.e. the ground state is degenerate, which also holds for $\Delta \epsilon/U = 3$: in this case, the states are coupled by a one-particle tunneling term. Then, by tuning the single-particle energies, as we approach $\Delta \epsilon/U = \pm 1$ or $\pm 3$, a peak in $\log_{10}(1 - F_{Fr})$ develops indicating that the perturbation does contain a one-particle tunneling term; likewise, a peak at $\Delta \epsilon/U = 0$ and $\pm 2$ develops if there are two-particle tunneling processes. This is illustrated in Fig. 3 which depicts $\log_{10}(1 - F_{Fr})$ in terms of $\Delta \epsilon/U$ for various even values of $n$. Note that the narrow peaks at $\Delta \epsilon/U = 0, \pm 2$, the signature of the two-particle tunneling, grow for increasing values of $n$. For odd values of $n$ the same argument applies, exchanging only the location of the peaks. Thus, by increasing $n$, the peaks associated with the two-particle tunneling processes become comparable to those associated to the one-particle tunneling processes; for big enough $n$ the distance between prominent neighboring peaks is halved. This result means that the fidelity freeze $F_{Fr}$ can also be maximized by tuning $\Delta \epsilon/U$.

Summarizing, we have found that the fidelity freeze from an initial symmetric coherent state is a sensitive quantity to two particle (and more) mode-exchange processes in the Bose-Hubbard model. This sensitivity can be controlled by two experimental parameters: the total atom number $n$ and the energy difference between modes $\Delta \epsilon/U$. In terms of $n$, $F_{Fr}$ displays a transition from a regime dominated by the one-particle exchange term, for small particle numbers, to the dominance of two-particle
FIG. 3: (Color online) Behavior of \( \log_{10}(1 - F_{Fr}) \) as a function of the energy difference between modes \( \Delta \epsilon \) scaled by the two-particle interaction coefficient \( U \) of the Bose-Hubbard model, Eq. \( \text{(2)} \). The 3D plot depict the appearance of a peak around \( \Delta \epsilon/U = 0, 2 \) which becomes noticeable as the particle number \( n \) increases.

The fidelity freeze can also be maximized by tuning \( \Delta \epsilon/U \). Our findings hold in the Fock regime of a double well potential, i.e. for \( J_i/U \ll 1 \). Ref. [33] explains how to reach the Fock regime (and others) by tuning simple experimental parameters; although the aspect ratio of the required confining geometries is inverted in relation to the traditional methods, novel experimental techniques may well be able to achieve them [24, 35]. Our findings combined with these methods could contribute to further improve atom interferometric techniques exploiting the non-linearities due to collisions [6] by minimizing the de-coherence effects associated to the quantum system itself. For example they could give rise to optimal methods for analysing the interference fringes imprinted by small energy differences between matter-waves [15]. Thus the fidelity freeze could become a rather useful tool for pushing the limits of atom interferometry.

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