Generalized Purity and Quantum Phase Transition for Bose-Einstein condensates in a Symmetric Double Well

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The generalized purity is employed for investigating the process of coherence loss and delocalization of the Q-function in the Bloch sphere of a two-mode Bose-Einstein condensate in a symmetrical double well with cross-collision. Quantum phase transition of the model is signaled by the generalized purity as a function of an appropriate parameter of the Hamiltonian and the number of particles \(N\). A power law dependence of the critical parameter with \(N\) is derived.

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Recently it has been pointed out that any bipartite and multiparticle entanglement measure can signalize the presence of a quantum phase transition (QPT) \([1, 2, 3]\) in many particle systems. Related to that, a subsystem-independent generalization of entanglement has been introduced based on coherent states and convex sets characterizing the unentangled pure states as coherent states of a chosen Lie algebra \([4]\). Such a notion of entanglement defined relative to a distinguished subspace of observables is pointed as particularly useful for classifying multiparticle entanglement and thus for QPT characterization. The generalized purity (GP) of the state relative to a certain distinguished subset of observables forming a local Lie algebra is directly related to the Meyer-Wallach measure \([5]\), and whenever a specific subsystem can be associated to the subset of observables the usual entanglement notion is recovered. On the other hand it has been demonstrated that the model describing a two mode Bose-Einstein condensate (BEC) in a symmetric double well (BECSDW) \([6]\), with cross-collisional terms \([7, 8]\) presents interesting dynamical regimes: The macroscopic self-trapping (MST) and Josephson oscillations (JO) of population \([9, 8, 9]\), both experimentally observed \([10]\). Recently a discussion of the transition from one regime to the other has been presented from the point of view of critical phenomena, as a continuous quantum phase transition problem in terms of the usual subsystem entropy \([11, 12, 13]\).

In this paper we apply the concept of GP in a BECSDW. Our purpose is twofold: \((i)\) We employ the GP relative to a chosen set of observables to quantify the quality of the semiclassical approach used in most of the treatments of BECSDW; \((ii)\) We characterize the quantum critical phenomena occurring in this model with the subsystem independent measure of quantum correlations \([4]\). The two mode approximated BECSDW has been well studied in the literature (see e.g. \([6, 9, 3]\)) as a model presenting a nonlinear self-trapping phenomena. More recently, the importance of the cross-collisional terms for large number of particles in the condensate \((N \gg 1)\) has been noticed \([7]\) and explored semiclassically with a time dependent variational principle (TDVP) based on coherent states \([8]\). For a fixed number of condensed particles \(N\), in order to explore the natural group structure of the model, we conveniently adopt the Schwinger’s pseudospin operators defined in terms of the creation and annihilation boson operators \(d^+_\pm, d^\pm\) on the approximated localized states \(|u\pm\rangle \ [6, 8]\): \(J_x \equiv \langle d^+_\pm d^-_\pm - d^\pm d^\pm\rangle/2\), \(J_y \equiv i\langle d^+_\pm d^-_\mp - d^\pm d^\mp\rangle/2\), and \(J_z \equiv \langle d^+_\pm d^-_\pm + d^\pm d^\pm\rangle/2\), where \(J = N/2\). In that form the two-mode BEC Hamiltonian writes as

\[
\hat{H} = 2 \left[ 2\Lambda(N-1) + \frac{\Omega}{2} \right] J_z + 2(\kappa - \eta) J^2_x + 4\eta J^2_z. \tag{1}
\]

where \(\Omega\) is the tunneling parameter, \(\kappa\) is the self-collision parameter of the condensate which is much larger than the so called cross-collision terms \(\eta\). \(\Lambda = \kappa \epsilon^3\), with \(\epsilon = \langle u_+ | u_- \rangle\). \(\Omega^2 \equiv 2[2\Lambda(N-1) + \Omega/2]\) is an effective tunneling parameter dependent on \(N\). The natural associated algebra of the model is \(su(2)\). In this form the Hamiltonian \([1]\) is a realization of the Lipkin-Meshkov-Glick model \([14]\), whose ground state entanglement has been investigated recently \([13]\) in the \(\eta = 0\) limit.

By means of a semiclassical method exploring \(SU(2)\) coherent states we have shown that for a sufficiently large \(N\) even a small amount of cross-collisional rate can change the dynamical regime of oscillations of the condensate from MST to JO \([8]\). The quantum and semiclassical MST and JO dynamics of the BECSDW are known to be qualitatively very similar \([6, 8]\) for large number of particles \((N \gg 1)\), except for the presence of collapses and revivals in the quantum time evolutions for the mean values of \(\langle J_x \rangle (t)\). This breaking of quantum-classical correspondence is due to decoherence \([15]\) introduced by quantum fluctuations, which drives the state of the system away from a coherent state. When we treat the semiclassical dynamics employing a TDVP \([15]\), we restrict the evolution of the state to a nonlinear subspace constituted only by the coherent states of \(SU(2)\) \([8]\). Such an evolution is exact for an initially coherent state only in the macroscopic limit of \(N \to \infty\) \([19]\). Also, in the TDVP approach we force the system wave function to be always localized in the phase space. From this point of view, the coherent states are the closest to the classical ones,
which are points in the classical phase space, and converges to them in the limit $N \to \infty$. The delocalization of the wave function (DWF) which goes along with the decoherence, is the responsible for the quantitative disagreement between the two dynamics [8], when collapses and revivals of expectation values of relevant observables happens with the DWF and consequent self-interferences occasioning the appearance of superposition states.

For a more complete analysis of the decoherence or of the quality of the semiclassical approximation, it becomes fundamental to have a good quantitative measure of the ‘distance’ of a given state to the subspace of the coherent states that give birth to the classical phase space. When the complete dynamics of the system is restricted to a space that carries an irreducible representation of $SU(2)$ (here this condition is satisfied due to the particle number conservation), there is a simple measure called GP of the form \[ \mathcal{P}_{su(2)} \] defined for $su(2)$ as

\[
\mathcal{P}_{su(2)}(\psi) = \frac{1}{J^2} \sum_{k=x,y,z} \langle \psi | J_k | \psi \rangle^2.
\] (2)

It is a good measure of decoherence, among other reasons, because it is invariant under a transformation of the group $SU(2)$ on the state $|\psi\rangle$: $\mathcal{P}_{su(2)}(U|\psi\rangle) = \mathcal{P}_{su(2)}(U|\psi\rangle)$, $\forall U \in SU(2)$. Thus, all the states connected by a $SU(2)$ transformation possesses the same purity. However, the most interesting property of $\mathcal{P}_{su(2)}$ – concerning the purpose of quantitatively compare the correspondence between the semiclassical and the exact quantum dynamics – is the fact that this measure has its maximum value at one, if and only if, the state is the coherent state closest to the classical state: $|\theta,\phi\rangle = R(\theta,\phi)(|J_+,J\rangle) = e^{-i\theta(J_x \sin \phi - J_y \cos \phi)}|J_+,J\rangle$. As soon as such a state moves away from the coherence, becoming delocalized in the phase space, the GP decreases monotonically to zero. Remark that the GP only has such properties clearly defined for pure states and, only in this case, it is a measure of existing quantum correlations of the state on the classical phase space.

We choose $|J,J\rangle_x \equiv |\theta = \frac{\pi}{2}, \phi = 0\rangle$ where $N = 100$ particles are in the same well, $\Omega = 1$ and $\kappa = \frac{2\Omega}{N}$. For this set of parameters it is known that choosing $\eta = \frac{\kappa}{10}$ the state is in the self-trapping region of the phase space, whereas for $\eta = \frac{\kappa}{10}$ it is outside the self-trapping region and thus in the JO regime [8]. In Fig. 1 we plot the GP, where the MST regime is in dashed line, and solid one for JO regime. In the MST regime the GP quickly drops down from 1 stabilizing at 0.9 for $\Omega t \approx 10$, indicating that the dynamics takes the state away from the subspace of CS. This plateau of purity coincides with the collapse region of population dynamics [8]. Note that close to $\Omega t = 30$ the purity shows small oscillations and in the region close to $\Omega t = 60$ the purity increases again until it practically recovers the value 1. At this instant the re-coherence of the state happens, being responsible for the revival of the oscillations of the population dynamics [8].

The agreement between the quantum and semiclassical results is due to the oscillation of the mean value of the generator $J_x$ in the MST, since the purity depends on the normalized square of such mean value. The oscillations of $\langle J_x \rangle$ around a non-zero value close to $J$ keeps also the value of $\mathcal{P}_{su(2)}$ close to its maximum possible value. In the JO regime for $\kappa = \frac{2\Omega}{N}$ and $\eta = \frac{\kappa}{10}$, the purity decays rapidly with the time, but in this case the decoherence is much stronger, and the purity reaches much lower values, not recovering to 1. Hence, this regime presents lower quantitative agreement between the quantum and classical evolutions, when compared to the MST regime. In this dynamical regime, the system does not recover high values of coherence. At a time close to $\Omega t = 250$ the state reaches its maximum re-coherence, but the GP value is still lower than 0.4. This result is expected because the classical orbit delocalizes much more on the Bloch sphere for this regime, and this entails a correspondingly large delocalization of the semiclassical Q-function on the sphere, $Q(\theta,\phi) = (\theta,\phi) |\psi\rangle \langle \psi|$, with $\rho = |\psi\rangle \langle \psi|$, during its evolution [8, 17]. The larger the region traveled by the trajectory in the phase space, larger the broadening of the distribution and smaller the coherence left on the state. Therefore, when the Hamiltonian has non-linear terms in the generators of the dynamical group, the semi-classical approximation has better quantitative accordance with the exact quantum results (for finite $N$) when the classical orbits sweep smaller ‘volume’ in the phase space. Since BECSDW model is integrable, we cannot analyze the decoherence due to chaotic trajectories. However, our results indicate that the semiclassical
method has lower validity for this type of trajectory that is less localized in the phase space.

Now we can take advantage of such qualities of the GP to characterize the quantum phase transition (QPT) [3]. The QPT is connected to a non-analyticity of the energy of the fundamental state of the system, when it is taken as a function of some real continuum parameter of the Hamiltonian [1] at zero temperature, in the thermodynamic limit $N \to \infty$. Generally speaking, the energy of the ground state in a finite system is an analytic function of any parameter of the Hamiltonian and only shows non-analyticity when $N \to \infty$, which then corresponds to an avoided level crossing. However, even when we are not allowed to take effectively such a limit, we still can observe the scaling of the properties of the system for increasing $N$ and infer about the occurrence of the QPT in the thermodynamic limit.

The BECSDW suffers a sudden change in its dynamics when $\kappa_c = \frac{\Omega}{N \sqrt{\kappa}}$ in the limit of no cross-collision terms and $N \gg 1$. With $\Omega, \kappa > 0$, such a transition of regime (JO to MST) does not occur at the ground state, but at the largest energy state for the value of parameter corresponding to the bifurcation in the classical phase space, which causes the appearance of a separatrix of motion.

Strictly speaking, the QPT is only characterized in the limit $N \to \infty$, thus our transition of dynamical regime (even if it occurred at the ground state) would only be considered as a \textit{bona fide} QPT in the exact classical limit. In Fig. 2, we have the Q-functions for the eigenstate of parameters $\kappa$ and $\eta$. Fig. 2a just shows the coherent state $|\theta = \pi, \phi\rangle = |J, J\rangle_z$, which is the maximum energy state of the non-interacting case $\kappa = \eta = 0$. In the absence of collisions, the most energetic eigenstate corresponds to the most localized state in the phase space, such that $P_{su(2)} = 1$. Increasing $\kappa$, but still not considering the cross-collision terms, the Q-function broadens along the $x$-axis, and consequently we expect the decreasing of the GP. At $\kappa = \kappa_c$, as shown in Fig. 2b, the state is greatly broadened, but still does not show a bifurcation; namely, the formation of two maxima in its distribution. This behavior is expected, since for finite $N$, the quantum transition parameter $\kappa_c^q(N)$ is slightly different from the value of transition $\kappa_c$ of the classical limit. But for increased $\kappa$, such as in Fig. 2c, for $\kappa = \frac{\Omega}{N}$, we see two maxima far apart along the $x$-axis as a signature of the bifurcation. The increase of the cross-collision has the opposite effect. For $\kappa = \frac{\Omega}{N}$, $\eta = \frac{\Omega}{N}$ the two peaks of the Q-function become closer, as in Fig. 2d.

![FIG. 2: (Color online) Q-function for the largest energy state of the $\hat{H}$ spectrum for several value of parameters $\kappa$ and $\eta$. Considering the number of particles $N = 100$ and $\Omega = 1$, we have the following values for the collision rates: (a) $\kappa = \eta = 0$; (b) $\kappa = \frac{1}{2\pi}, \eta = 0$; (c) $\kappa = \frac{\Omega}{N \sqrt{\kappa}}, \eta = 0$ and (d) $\kappa = \frac{1}{10}, \eta = \frac{\Omega}{N}$.

Our results for the phase space distribution of the maximum energy state are confirmed as we analyze the behavior of the GP as a function of the self-collision parameter and the number of particles, as shown in Fig. 3, neglecting the cross-collisions. The GP initially decreases slowly with $\frac{\kappa N}{\Omega}$, independent of the value of $N$, corresponding to the region where the distributions broadens along the $x$-axis. However, close to $\frac{\kappa N}{\Omega} = \frac{1}{2}$, the GP begins to decrease quickly and, although smoothly, the lowering of its value is more and more steep as we increase $N$. This behavior of $P_{su(2)}$ suggests us a strong dependence between the derivative of the GP with respect to $\frac{\kappa N}{\Omega}$ and the number of particles. In Fig. 4 we show the derivative of the GP with respect to the normalized self-collision parameter $\frac{\kappa N}{\Omega}$ for various values of $N$. For an increasing number of particles, we see the minimum value of the derivative of $P_{su(2)}$ to move to the left side, closer to the classical critical value (0.5), and also the minimum becomes more pronounced. We define the value of

![FIG. 3: (Color online) GP of $su(2)$ for the largest energy eigenstate as a function of normalized self-collision parameter and the number of particles, with cross-collision rate $\eta = 0$.

![FIG. 4: (Color online) GP of $su(2)$ for the largest energy eigenstate as a function of normalized self-collision parameter and the number of particles, with cross-collision rate $\eta = 0$.](image)
\[ \kappa N \] at the minimum of the derivative of \( \text{GP} \) as the critical value of the quantum dynamical transition \( \kappa^q(N) \). It is already clear that the value of \( \kappa^q(N) \) is brought closer to the classical transition value \( \kappa_c = \frac{\Omega}{2N} \) for increasing \( N \), but we still need to characterize how this approximation happens. The values of \( \ln \frac{N(\kappa^q - \kappa_c)}{\Omega} \) from the curves in Fig. 4 suggest a power law between \((\kappa^q - \kappa_c)\) and \( N \). A linear interpolation of the data points gives \( \kappa_c - \kappa_c = \frac{\Omega}{N}e^{0.31 \pm 0.05}N^{-0.657 \pm 0.009} \propto N^{-1.657 \pm 0.009} \). It is evident that \( \kappa^q \to \kappa_c \) as \( N \to \infty \).

In conclusion we considered the \( \text{GP} \) to analyze the dynamics of coherence loss of initially coherent state for the BECSDW model. In the MST regime the \( \text{GP} \) remains high without significant decoherence. For the JO regime, on the other hand, we have seen that the first decay of the \( \text{GP} \) was in a similar time scale to the MST one, being the decoherence much more significant. In the JO regime no considerable re-coherence can be achieved and the \( \text{GP} \) correspondingly has a much lower value than in the previous regime at this time. Since the coherent state represents the closest to the classical state, the value of \( \text{GP} \) enabled us to estimate the quality of the semiclassical approximation at each time in both regimes. Moreover we have employed the \( \text{GP} \) as a tool for characterizing a QPT in the same model. We have shown for finite number of particles (\( N < \infty \)) the bifurcation of the \( \text{GP} \) as the self-collision parameter \( \kappa \) becomes larger than a critical value \( \kappa^q(N) \). Also, we have shown the suppression of cross-collisions between the particles in different wells. By increasing the number of particles \( N \), the \( \text{GP} \) has shown a more and more steeper behavior near the critical value of \( \kappa N \); moreover, its value has tended to the known classical value \( \kappa_c = \frac{1}{2} \) as \( N \to \infty \). Finally we have shown that \( \kappa^q - \kappa_c \) is consistent with a power law in \( N \). Therefore, the \( \text{GP} \) for this model is an excellent measure for both to indicate the dynamical loss of coherence of initially coherent state and to indicate the QPT. When a state suffers fundamental changes resulting from the QPT, its \( \text{GP} \) must follow its behavior, because it has all the information about its coherence and the degree of localization over the phase space.

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[18] Here decoherence is employed as being far from the classical situation, not to be confused with the more frequently used sense where the classical character is induced by a coupling with the environment.
[19] This is also true when the Hamiltonian is linear in the generators of the dynamical group. Namely this would be the present case only in the limit of non-interacting particles (\( \kappa = 0 = \eta \)).