Global phase space of coherence and entanglement in a double-well Bose-Einstein condensate

Holger Hennig,1 Dirk Witthaut,2 and David K. Campbell1

1Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA
2Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany
3Department of Physics, Boston University, Boston, Massachusetts 02215, USA

(Received 4 June 2012; published 12 November 2012)

Ultracold atoms provide an ideal system for the realization of quantum technologies but also for the study of fundamental physical questions such as the emergence of decoherence and classicality in quantum many-body systems. Here, we study the global structure of the quantum dynamics of bosonic atoms in a double-well trap based upon the Bose-Hubbard Hamiltonian and analyze the conditions for the generation of many-particle entanglement and spin squeezing which have important applications in quantum metrology. We show how the quantum dynamics is determined by the phase-space structure of the associated mean-field system and where true quantum features arise beyond this “classical” approximation.

Maintaining and controlling the coherence of quantum systems over time is one of the major challenges in contemporary physics. Low-temperature quantum gases trapped in optical lattices are an important instance of this challenge, for they provide versatile testbeds both for idealized models of exotic solid-state systems and for applications in quantum optics and quantum information processing [1–4]. A Bose-Einstein condensate (BEC) loaded in two linearly coupled wells, called a “BEC dimer” or “bosonic Josephson junction” [5], is a particularly appealing case, as its quantum behavior is both theoretically tractable [6–9] and experimentally accessible. In particular, BEC dimers have been shown to allow coherent manipulation of quantum states even on an atom chip, enabling matter-wave interferometry [10], long phase coherence times and number squeezing [11–13], and proposed chip-based gravity detectors [14]. Related questions have been addressed in the context of the mathematically equivalent Lipkin-Meshkov-Glick model [15].

For large atom numbers, the coarse dynamics of the BEC dimer is well described by a “classical” mean-field approximation. Recent experiments have precisely mapped out the classical phase-space structure [16,17], showing macroscopic quantum oscillations as well as the emergence of self-trapped states through a “classical” bifurcation. Recent theoretical studies have focused on strategies to prepare highly entangled states through a “classical” bifurcation. Recent theoretical and insights into true quantum effects beyond the mean-field or semiclassical approaches.

Quantum and semiclassical dynamics. The coherent dynamics of the BEC dimer is given by the two-mode Bose-Hubbard Hamiltonian (BHH)

\[ H = -J \left( \hat{a}_1^\dagger \hat{a}_2 + \hat{a}_1 \hat{a}_2^\dagger \right) + \frac{U}{2} \left( \hat{a}_1^\dagger \hat{a}_1 \hat{a}_2^\dagger \hat{a}_2 \right), \] (1)

where \( \hat{a}_j \) denotes the annihilation of one bosonic atom in state \( j \). The modes can be realized by two sites in a double-well trap [23,24] or two internal states of the atoms [17]. The tunneling rate \( J \) and the on-site interaction \( U \) can be tuned individually, e.g., via a Feshbach resonance or by changing the trapping potential [1,13,17,25–27]. We set \( \hbar = 1 \), thus measuring all energies in frequency units and assume \( J = 10 \) s\(^{-1} \), which is a common experimental setting [13,17,27], and a total number of \( N = 40 \) atoms. We study the symmetric quantum dimer. In the presence of a small asymmetry of the double well, the classical fixed points (see below) would be slightly shifted. Since we qualitatively and quantitatively map EPR entanglement and the condensate fraction to the purely classical dynamics (using LiDA), it is strongly expected that our general findings are valid in the presence of a small asymmetry.

The mean-field counterpart of the Bose-Hubbard dimer is a two-mode GPE. This equation can be rewritten as an integrable classical Hamiltonian system with the Hamiltonian [28]

\[ H_2(z,\varphi) = \frac{\Lambda z^2}{2} - \sqrt{1 - z^2} \cos(\varphi). \] (2)

The mean-field (classical) phase space consists of the two conjugate variables, the relative phase \( \varphi = \varphi_1 - \varphi_2 \in [0,2\pi) \) between the two wells and the population imbalance \( z = (N_1 - N_2)/N \in [-1,1] \), where \( N_{1,2} \) denote the number of atoms in each well and \( N = N_1 + N_2 \) is the total atomic population [28]. The classical trajectories follow the lines of constant (conserved) energy \( H_2(z,\varphi) = \text{const} \). They are
determined by the initial position \((\varphi_0, z_0)\) in phase space and the ratio of the interaction and the tunneling energy \(\Lambda = UN/(2J)\).

The GPE implicitly assumes a pure BEC at all times. Some quantum features beyond this rough approximation, in particular, the quantum mechanical spreading over time, can be included if a quantum state \(|\Psi\rangle\) is represented by a (quantum) phase-space density such as the Husimi function \(Q(\varphi, z) = |(\varphi, z)|^2\) instead of a single trajectory. Here, \(|\varphi, z\rangle\) denotes an atomic coherent state [29], which is nothing but a pure BEC. The dynamics of the Husimi function follows a classical Liouville equation with the Hamiltonian (2) plus quantum correction terms vanishing as \(1/N\) [22]. In the semiclassical LiDA [22] we thus represent a quantum state by an ensemble of trajectories, whose initial positions are distributed according to the Husimi function of the initial quantum state. With increasing atom number \(N\) the system converges to the semiclassical limit, i.e., the differences of the full quantum dynamics and the semiclassical LiDA vanish.

**Global phase-space structure.** We analyze the global phase-space structure of the Bose-Hubbard dimer with special respect to its classical and quantum properties. Therefore, we consider the dynamics of an initially pure BEC as a function of the parameters \(z_0\) and \(\varphi_0\) with a focus on the condensate purity and entanglement. The purity is measured by the condensate fraction \(c_t(\varphi, z)\) defined as the maximum eigenvalue of the reduced single-particle density matrix \(\rho_{ij} = \langle a^*_i a_j \rangle/N\) [9,22,30]. A related GPS approach was introduced in terms of the phase-space entropy [31].

The GPS of the Bose-Hubbard dimer is shown in Fig. 1, where the condensate fraction \(c_t(\varphi, z)\) at time \(t = 1\) s is plotted as a function of the initial state \(|\varphi_0, z_0\rangle\) for three different values of \(\Lambda\). The corresponding classical mean-field dynamics is overlaid as solid black lines. For \(\Lambda < 1\), the atoms show Rabi oscillations between the wells with stable fixed points at \(F_1 = (0, 0)\) and \(F_2 = (\pi, 0)\). According to the average phase \(\bar{\varphi}\), the oscillations are referred to as “zero-phase” or plasma oscillations \((\bar{\varphi} = 0)\) around \(F_1\) and “\(\pi\)-phase” oscillations \((\bar{\varphi} = \pi)\) around \(F_2\). The classical dynamics undergoes a bifurcation at \(\Lambda = 1\), separating the Rabi \((0 < \Lambda < 1)\) and Josephson \((\Lambda > 1)\) regimes. The fixed point \(F_2\) becomes hyperbolically unstable for \(\Lambda > 1\), bifurcating into two self-trapping (ST) fixed points at \(F_{ST} = (\pi, z_{ST})\), where \(z_{ST} = \pm \sqrt{1 - 1/\Lambda^2}\) [28]. In addition to \(\pi\)-phase ST with average phase \(\pi\) [Fig. 1(b)], also “running phase” ST appears for \(\Lambda > 2\) [see Fig. 1(a)].

The GPS for the condensate fraction \(c_t(\varphi, z)\) in Fig. 1 shows that lines of equal \(c_t(\varphi, z)\) mimic the classical trajectories, thus reflecting zero- and \(\pi\)-phase oscillations and fixed points as well as ST. A drastic drop in the condensate fraction is observed especially near the classical separatrices, demonstrating deviations from a pure BEC and thus the failure of a mean-field description. Notably, this loss of coherence is not strongest at the unstable fixed point (see Fig. 1).

The correspondence of quantum and classical phase-space structure is more than a qualitative coincidence. In Figs. 2(a) and 2(b) we compare the quantum results (based upon the BHH) for the minimum condensate fraction with the prediction of the semiclassical LiDA. The good agreement reveals that the loss of quantum coherence \(c_t(\varphi, z)\) can be mostly attributed to the classical spreading of Husimi function. Around a stable fixed point neighboring trajectories remain close for all times, such that there is no spreading.

But why does the quantum coherence remain reasonably high near the unstable fixed point? We recall that Eq. (2) can be mapped to a pendulum with variable length \(l(z) = \sqrt{1 - z^2}\) and angular velocity \(\dot{\varphi} = \psi\). Within that picture, the unstable fixed point \(F_2 = (\pi, 0)\) is reached when the pendulum is in its upright position with no angular velocity. Close to \(F_2\), the classical dynamics slows down asymptotically (“freezes”); therefore spreading near the unstable fixed point is slow. Moreover, the pendulum slows down when moving towards \(F_2\) and accelerates when moving away, which breaks \(S\) symmetry. On the contrary, close to the separatrix (corresponding to the energy of \(F_2\)), the classical dynamics leads to delocalization in phase space, which induces decoherence of a many-particle state [22,31].

To study to what extent these features can be captured in a time-independent framework, we analyze the overlap of \(|\varphi, z\rangle\) with an eigenstate \(|E_n\rangle\) of the Bose-Hubbard dimer.
entanglement, a simple criterion reads

(b) For min[c(0.85π, z)] the condensate fraction min[c(0.85π, z)] in the time interval 0 < t < 0.5 s. The point (0.85π, 0) is near the hyperbolic fixed point. The LiDA reproduces S-symmetry breaking, but deviates from the quantum results near the hyperbolic fixed point and the separatrices (dashed vertical lines). (For min[c(0, z)] the LiDA deviates from the quantum dynamics for |z| ≲ 0.8, i.e., near the separatrices (which are located at z = ±0.8, dashed lines). (d) Large c in the vicinity of the classical fixed points is reproduced qualitatively by a time-independent measure. The color code shows A = maxₙ |⟨ψ(ϕ,z) | Eₙ⟩| for (c) A = 5 and (d) A = 1.5.

Figures 2(c) and 2(d) show the maximum overlap A(ϕ, z) = maxₙ |⟨ψ(ϕ,z) | Eₙ⟩| for the same parameters as in Figs. 1(a) and 1(b). The overlap is high at the stable fixed points and minimal along most parts of the separatrices (cf. Refs. [32–34]). This reveals one possible mechanism to maintain long-time coherence of a BEC: If the overlap approaches unity, the initial state is almost stationary such that the condensate fraction remains virtually constant. This is consistent with (but the converse of) the results reported in Refs. [22,31], where it was shown that delocalization in phase space induces decoherence of a quantum state. Moreover, there is also an eigenfunction localized around the unstable fixed point E₂, which explains the surprisingly slow decoherence at this point. However, several quantum features depicted in the GPS, such as the symmetry breaking, are not reproduced by A(ϕ, z), indicating that these are of dynamical origin.

Entanglement. A distinguishing feature of experiments with two-mode BECs is that the quantum state can be manipulated with astonishing precision. In particular, the atoms can be strongly entangled, with applications in precision quantum metrology [13,35,36]. For the important special case of EPR entanglement, a simple criterion reads E > 0, where E = |⟨d₁†d₂⟩|² − |⟨d₁†d₂⟩|² [19,20]. The GPS picture for the EPR entanglement is shown in Figs. 3(a) and 3(b). The measure $Eₜ(ϕ,z)$ again closely mimics the classical phase-space trajectories. At time t = 1 s, entanglement $E > 0$ is found only near the classical ST fixed points. Movies showing the evolution of $Eₜ(ϕ,z)$ for t ∈ [0,3] s can be found in the Supplemental Material [37]. Strikingly, the GPS for entanglement unveils the following behavior: If entanglement appears on time scales that are long compared to the period of the plasma oscillations, then entanglement is concentrated around the fixed points in phase space.

Given the apparent similarity of the GPS for E and the condensate fraction c, we ask, how is E related to c? By approximating $⟨d₁†d₁⟩^2 ≈ ⟨d₁†d₁⟩$ we find a semiclassical measure $E_c = |⟨d₁†d₂⟩|^2 − |⟨d₁†d₂⟩|^2 = N²( c² − c )$. The GPS for $E_c$ in Fig. 3(c) shows a remarkable qualitative agreement with the exact quantum results for E. In Fig. 3(d) we report the temporal evolution of E and $E_c$ of the state $|0.2,0⟩$, which shows surprisingly good agreement except for an offset. However, as $E_c ≲ 0$ by definition, it does not serve as an entanglement criterion.
Spin squeezing indicates a form of entanglement which is particularly important for quantum metrology [13,35]. A state is spin squeezed if the quantum uncertainty in a Bloch sphere representation is smaller than that of an atomic coherent state, i.e., a pure BEC. This representation is defined via the operators $\hat{\sigma}_x = \frac{1}{2}(\hat{a}_1^2\hat{a}_2 + \hat{a}_2^2\hat{a}_1)$, $\hat{\sigma}_y = \frac{1}{2}(\hat{a}_1^2\hat{a}_2 - \hat{a}_2^2\hat{a}_1)$, and $\hat{\sigma}_z = \hat{a}_1^2\hat{a}_2^2$, which form an angular momentum algebra [22,29,30]. A quantum state is spectroscopically squeezed, if [36]

$$\xi^2 := \frac{N(\Delta J_n)}{\langle J_n \rangle^2} < 1. \quad (3)$$

Here, $\hat{J}_n = n_1 \hat{J}$ is the projection of the total angular momentum operator $\hat{J}$ onto $n_1$, where $n_{1,2,3}$ are mutually orthogonal unit vectors and $\Delta \hat{J}_n$ is the uncertainty of $\hat{J}_n$. In Fig. 3(e) we report the dynamical evolution of $\xi^2$ for an initially pure BEC $|0,2,0\rangle$, in excellent agreement with $E(t)$ [Fig. 3(d)], including the entanglement revival at $t \approx 3\ s$.

Discussion. While chaotic classical dynamics typically leads to fast (exponential) decay of the coherence of a many-particle state [38], little is known about the coherence of quantum self-trapped states, especially in higher dimensions, where the classical counterparts are (quasi)periodic orbits, although some insight is provided by semiclassical approaches beyond the mean-field limit [39–41]. Figure 2 reveals one aspect of the coherence of self-trapped states. For $z$ near $\pm 1$ the many-particle state is close to a pure condensate, whereas the condensate fraction drops drastically well before the separatrix (dashed line) is reached. Hence, ST is a mechanism to preserve coherence of many-particle states, which is further confirmed by the results reported in Figs. 1(a) and 1(b). In contrast, in the vicinity of the separatrix, the condensate fraction falls off sharply.

We have analyzed the connection between quantum observables of the BEC dimer and the structure of the underlying classical phase space, including fixed points, separatrices, and ST. The question remains: How well do our results carry over beyond the Bose-Hubbard model? Recent numerical studies beyond the Bose-Hubbard model (including higher-lying states in the individual wells) [42,43] show that ST is only present as long as the system remains coherent. Hence, there is evidence that our results do reflect a fundamental relation between ST and coherence of Bosonic quantum systems.

In larger optical lattices, the self-trapped states correspond to “discrete breathers” or “intrinsic localized modes” [44–49]. These correspond to classical trajectories which are practically embedded on a two-dimensional torus in the high dimensional phase space and are thus (quasi)periodic in time [45,46,50,51]. Thus, discrete breathers involve localization in phase space. Moreover, discrete breathers become attractive fixed points in presence of dissipation [45,52,53], and occur in a variety of physical and biochemical systems [44,46,47]. Just as delocalization in classical phase space leads to decoherence [22,31], we expect that discrete breathers are candidates to support long-lived coherent and possibly entangled many-body states even in complex dissipative systems, such as biomolecular systems.

Acknowledgments. We thank Ted Pudlik for comments. H.H. acknowledges financial support by the Deutsche Forschungsgemeinschaft (DFG Grant No. HE 6312/1-2). D.K.C. thanks Boston University for partial support of this research and the Kavli Institute for Theoretical Physics for its hospitality during the completion of this work.
[37] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevA.86.051604 for movies showing the time evolution of the GPS for EPR entanglement $E(t)$ for $\Lambda = 5$ and $\Lambda = 0.5$.