Delocalization to self-trapping transition of a Bose fluid confined in a double-well potential: an analysis via one- and two-body correlation properties

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Abstract
We revisit the delocalized to self-trapping transition in an interacting bosonic fluid confined in a double-well potential in the context of full quantum calculations. We first study one- and two-body properties in the energy eigenstates to determine the transition as a function of the energy of the fluid. This occurs provided the interparticle interaction is above a critical or threshold value. Next, we analyse the evolution in time of the same observables in a set of coherent states to show that the \(N\)-particle Bose fluid reaches stationary states, whose expectation values turn out to coincide with those in the eigenstates. This stationary or collapsed state alternates with recurrent revivals. Here we show that the time spent in the stationary state increases with the number of particles, relatively to the time during the revivals. This stationarity property is in severe contrast with that of mean-field states since these always appear as coherent oscillations either for delocalized or self-trapped states.

1. Introduction
The experimental realization of a single bosonic Josephson junction in two weakly linked Bose–Einstein condensates (BECs) has revealed fundamental features of the dynamical nature of an ultracold interacting Bose gas in a double-well potential [1]. The atomic transport has shown the existence of Josephson tunnelling or macroscopic quantum self-trapping regimes depending on the interatomic interactions and on the initial populations in the wells. These opposite states are similar to the well-known superfluid and Mott insulator states observed in optical lattices [2, 3] in the sense that the quantum transition among them is the result of the nonlinear condensate self-trapping interactions.

The theoretical analysis of the double-well system has mainly been based on the two-mode approximation [4–17]. Besides providing a fairly good description of the experimental situation [1], this model has been extensively studied on its own, specially within a mean-field or semiclassical approximation. This model has lead to significant understanding of the richness of the physical problem at hand; additionally, it can incorporate asymmetric two-well potentials and external time-dependent driving fields [10]. One should also point out the relevance of this model in analysing problems in other fields, such as in nonlinear optics [18, 19].

Beyond the mean-field approximation, this model is amenable to numerical full quantum calculations, so far up to \(N = 1000\) particles [4, 10, 14–17]. The mean field, by approximating the \(N\)-body dynamics by a set of nonlinear coupled dynamical equations, is limited and incomplete since it describes the evolution of the expectation values of one-body...
operators only. In contrast, from the full quantum description one may, in principle, enquire about the dynamics of one-, two-, three- and up to N-body properties. Due to the relative simplicity of the present model one can calculate either the full N-body wavefunction for a pure state or the full N-body density matrix for a mixed state (for a system up to \( N = 10000 \) particles, say). Thus, full information of the state of the system may be obtained. However, from a macroscopic point of view, most of the measurable thermodynamic and/or many-body properties, such as energy, temperature and Green’s functions in general, are given in terms of one- and two-body operators [20]. These in turn are exhaustively described by the one- and two-body reduced density matrices. Although we are able to calculate the complete one- and two-body density matrices from the exact solution, here for purposes of showing our main points we shall limit our study to the following measurable quantities: the number of particles in one of the wells, given by the expectation value of a one-body operator \( \hat{N}_1 \), and a tunnelling correlation function, the expectation value of a two-body operator \( \hat{J}_x \hat{J}_x \).

We proceed as follows. Since we are dealing with a macroscopic system, we choose to describe the state of the system by specifying the number of particles \( N \) and the expectation value of the energy \( \varepsilon \). For this to be meaningful, we must limit ourselves to states whose energy mean-square deviation is small, in other words, to states localized in energy. For our analysis we choose both the energy eigenstates and a well-known family of coherent states [21, 22] such that the energy requirement is satisfied. We point out here that the particular state with all particles initially in one of the wells, analysed in most of the studies with full quantum solutions [10, 11, 14–16], belongs to the family of such coherent states.

We first analyse the expectation values of the chosen operators, \( \hat{N}_1 \) and \( \hat{J}_x \hat{J}_x \), in the energy eigenstates and study their values as a function of the interaction strength \( \Lambda = NU/\hbar \alpha \), where \( \Delta \) is the tunnelling frequency and \( U \) is the two-body interaction. We find that the expectation values of \( \hat{N}_1 \) and \( \hat{J}_x \hat{J}_x \) in the eigenstates signal the transition from delocalization to self-trapping. This behaviour is summarized in a phase diagram. The main result being that there exists a critical value of the interaction, such that if the interaction is greater than this value, the self-trapping transition occurs as a function of the energy of the system. Then we make a brief review of the mean-field stationary solutions to contrast and point out similarities. In particular, we show that the phase diagram separating delocalized from self-trapped states is essentially the same for exact and mean-field calculations [10].

Next we turn our attention to the study of the dynamics of states that initially belong to the mentioned family of coherent states. A typical behaviour is that the time-dependent expectation values \( \langle \hat{N}_1 \rangle \) and \( \langle \hat{J}_x \hat{J}_x \rangle \) oscillate for a brief period of time, the former with the same frequency as that predicted by mean-field theory. Then, these oscillations collapse to a stationary value for a longer period of time followed by revivals. This stationary value depends on the expectation value of the energy and on the interaction parameter \( \Lambda \). That is, the stationary value may correspond to a delocalized or to a self-trapped state. It turns out that such a stationary value of the given operator in the coherent state agrees with its expectation value in the energy eigenstate with the same energy. We find that the mean field shows deviations from those values, the departure being larger as the interaction is increased.

The phenomenon of collapse and revivals of the expectation values of few-body operators in many-body time-dependent states has been recorded and analysed by many authors, see e.g. [7, 8, 10–16, 23]. Here, we would like to emphasize an additional point which is the fact that as the number of particles is increased, the time spent in the revival regions and the time spent in the stationary region both increase. However, the ratio of the latter to the former also increases, such that most of the time is spent in the stationary region, regardless of the size of the interaction and of the initial state. For this reason we call those ‘statistically stationary’ states, in addition to the fact that their expectation values agree with those in the truly stationary energy eigenstates. One can certainly argue that this is a form of intrinsic decoherence [23], shown by properties of few bodies within a system of many particles.

In the next section we introduce the Hamiltonian of the system as well as the quantities to be analysed and discuss the results for both the energy eigenstates and the mean-field counterparts. The third section deals with the dynamics of the coherent states and the non-stationary mean-field evolution. We conclude with brief remarks regarding our main results.

2. The model, observables and eigenstate properties

We model the interacting quantum fluid confined in the double well through the Bose–Hubbard Hamiltonian considering the two-mode approximation [4]

\[
\hat{H} = -\frac{\hbar \Delta}{2} (\hat{b}_1^\dagger \hat{b}_2 + \hat{b}_2^\dagger \hat{b}_1) + U (\hat{b}_1^\dagger \hat{b}_1^\dagger \hat{b}_2 \hat{b}_2 + \hat{b}_2^\dagger \hat{b}_1 \hat{b}_1^\dagger \hat{b}_2),
\]

(1)

where \( \Delta \) is the tunnelling frequency of the two lowest energy modes in a symmetrical two-well potential and \( U = 4\pi \hbar^2 a / m \) represents the effective particle–particle interaction strength written in terms of the (positive) s-wave scattering length \( a \). We shall specify the different regimes by the adimensional interaction parameter \( \Lambda = NU/\hbar \Delta \). We use units with \( \hbar = \Delta = m = 1 \).

As it has already been established, both from mean-field and full quantum calculations, the system described by Hamiltonian (1) exhibits a transition from delocalized oscillations to a self-trapping regime. This transition has been described to occur as either when the parameter \( \Lambda \) is increased from zero to above a critical value \( \Lambda_c \) for a fixed initial condition, or for a fixed value of \( \Lambda > \Lambda_c \) by varying the initial state, which is equivalent to varying the energy of the system. As a matter of fact, the experiment by Albiez et al [11] using Bose atoms at very low temperatures reports the observation of a self-trapped state as a function of the initial population imbalance.

3 This model is also a particular case of the so-called LMG model in nuclear physics [24]. For recent developments in the eigenstate structure of such a model, see [25] and [26].
In this section we shall analyse the behaviour of the one- and two-body observables on the quantum eigenstates along the transition and we shall also briefly review the corresponding predictions of the mean field. We will point out their similarities and discrepancies. The next section will be devoted to study the full time quantum evolution of the quasiclassical coherent states along the transition.

Within a quantum calculation one can obtain the full \(N\)-body wavefunction \(\psi_N(t)\) and the density matrix \(\hat{\rho}^{(N)}(t) = \langle \psi_N(t) | \psi_N(t) \rangle\). From the latter, one may further find the reduced one- and two-body density matrices, \(\hat{\rho}^{(1)}\) and \(\hat{\rho}^{(2)}\), whose matrix elements are given by

\[
\rho^{(1)}_{ab} = \text{Tr}(\hat{b}_a \hat{\rho}^{(N)} \hat{b}_b) \tag{2}
\]

and

\[
\rho^{(2)}_{ab} = \text{Tr}(\hat{b}_a \hat{b}_b \hat{\rho}^{(N)} \hat{b}_a^{\dagger} \hat{b}_b^{\dagger}) \tag{3}
\]

with the subindices \(a\) and \(b\) taking the values 1 and 2, and \(a = \{\mu \nu\}\) and \(b = \{\kappa \eta\}\), that is, the values \(11, 12\) and \(22\). Knowledge of these two operators suffices to determine all one- and two-body properties of the system. However, even though we can calculate all the matrix elements of \(\hat{\rho}^{(1)}\) and \(\hat{\rho}^{(2)}\) as a function of time, we find it more illustrative to limit ourselves to the analysis of two properties, one is the number of particles in well 1, namely

\[
\hat{N}_1 = \hat{b}_1^{\dagger} \hat{b}_1, \tag{4}
\]

a one-body operator, and the other is a ‘tunnelling correlation’,

\[
\hat{C} = \hat{J}_x \hat{J}_x, \tag{5}
\]

a two-body operator, with \(\hat{J}_x = (\hat{b}_1^{\dagger} \hat{b}_2 + \hat{b}_2^{\dagger} \hat{b}_1)/2\) the tunnelling operator.

To analyse the properties of the eigenstates of the system, we numerically solve the eigensystem, \(\hat{H}(\Lambda)|\phi_n(\Lambda)\rangle = \epsilon_n(\Lambda)|\phi_n(\Lambda)\rangle\), where the dependence of different set of eigenstates and eigenvalues on \(\Lambda\) has been indicated. For \(N\) particles there are \(N + 1\) eigenstates, the energy of the system being finite and bounded by the lowest \(\epsilon_0(\Lambda)\) and largest \(\epsilon_N(\Lambda)\) eigenenergies. In figures 1 and 2 we show the expectation values of \(\hat{N}_1\) and \(\hat{C}\) in the energy eigenstates, namely \(\langle \hat{N}_1(\Lambda) \rangle_n = \langle \phi_n(\Lambda) | \hat{N}_1 | \phi_n(\Lambda) \rangle\) and \(\langle \hat{C}(\Lambda) \rangle_n = \langle \phi_n(\Lambda) | \hat{C} | \phi_n(\Lambda) \rangle\) as a function of the eigenenergy \(\epsilon_n(\Lambda)\) of the corresponding eigenstate, for three illustrative values of the interaction, \(\Lambda = 0.1, \Lambda = 1.0\) and \(\Lambda = 10\).

From figures 1 and 2 we can appreciate the behaviour of the observables \(\hat{N}_1\) and \(\hat{C}\) on the energy eigenstates and at the same time the transition to self-trapping as \(\Lambda\) is varied. For \(\Lambda = 0.1\) all the stationary states show, on the one hand, \(\langle \hat{N}_1 \rangle_n = N/2\) while \(\langle \hat{C} \rangle_n\) shows a simple continuous behaviour. For obvious reasons, we call delocalized states those with \(\langle \hat{N}_1 \rangle_n = N/2\). Thus, for \(\Lambda = 0.1\) all states are delocalized. For \(\Lambda = 1.0\) and \(\Lambda = 10.0\) a transition is observed. One finds that there exists a ‘critical’ energy \(\epsilon_c(\Lambda)\), above which the average number of particles deviates from \(N/2\), i.e. \(\langle \hat{N}_1 \rangle_n \neq N/2\). These are the self-trapped states, which appear as a breaking of the symmetry \(1 \leftrightarrow 2\) of Hamiltonian (1). In the case of the tunnelling correlation \(\langle \hat{C} \rangle_n\) the transition is signaled by a cusp at \(\epsilon_c(\Lambda)\). We also performed

\[\text{Figure 1. Eigenstate expectation value of the particle population in well 1 } \langle \hat{N}_1 \rangle_n \text{ as a function of the energy eigenvalues } \epsilon_n \text{ for } N = 1000 \text{ and } \Lambda = 0.1, \Lambda = 1.0 \text{ and } \Lambda = 10.\]

\[\text{Figure 2. Eigenstate expectation value of the two particle correlation } \langle \hat{C} \rangle_n \text{, as a function of the energy eigenvalues } \epsilon_n \text{ for } N = 1000 \text{ and } \Lambda = 0.1, \Lambda = 1.0 \text{ and } \Lambda = 10.\]

The eigensystem \(\hat{H}(\Lambda)|\phi_n(\Lambda)\rangle = \epsilon_n(\Lambda)|\phi_n(\Lambda)\rangle\) was numerically solved by means of Fortran and Mathematica diagonalization subroutines. The time evolution of an arbitrary initial state, \(|\psi(t)\rangle = \sum_{n \mu} a_{\mu}|\phi_n(\Lambda)\rangle\), was performed, both, by direct evaluation of \(|\psi(t)\rangle = \sum_{n \mu} a_{\mu} \exp(-i\epsilon_n(\Lambda)t)|\phi_n(\Lambda)\rangle\) with Mathematica, and by a finite-difference method within a Fortran code.
Figure 3. Phase diagram $\varepsilon/N$ versus $\Lambda$ for $N = 1000$ particles. The allowed states are those within the (blue) solid lines, $\varepsilon_{\text{MF}}(\Lambda)$ and $\varepsilon_N(\Lambda)$. The (red) dotted line is the transition from delocalized to self-trapped states, $\varepsilon_N(\Lambda)$ for $\Lambda > \Lambda_c \approx 0.539$, see the inset. The states with energy greater than $\varepsilon_N(\Lambda)$ are self-trapped.

calculations with $N = 10^4$ and we found that the difference with $N = 1000$ is almost indistinguishable, except very near the transition. In figure 1 note that there are two isolated points near the transition; for $N = 10^4$ there are few more isolated points around the transition. We may speculate that as $N$ grows without bound, the line in figure 1 may become continuous; yet, the results up to $N = 10^4$ show an apparent discontinuous transition. This aspect deserves further research.

The transition is best summarized in the phase diagram of figure 3. This was obtained by the diagonalization of Hamiltonian (1), considering $N = 1000$ particles, for values of $\Lambda$ ranging from $0.0 \leq \Lambda \leq 10.0$ in steps of 0.01. For each set of eigenstates we found the value $\varepsilon_N(\Lambda)$ where the delocalized to self-trapping transition occurred. This is the (red) dotted line in figure 3. The (blue) solid lines correspond to the lowest and highest eigenenergies for each value of $\Lambda$, namely $\varepsilon_0(\Lambda)$ and $\varepsilon_N(\Lambda)$. Hence, for $\varepsilon_0(\Lambda) \leq \varepsilon_N(\Lambda)$ the state $|\phi_0(\Lambda)\rangle$ is delocalized, while it is self-trapped for $\varepsilon_0(\Lambda) \geq \varepsilon_N(\Lambda)$.

We further observe that there exists a critical value of the interaction $\Lambda_c$ below which there is no transition. For $N = 1000$ we numerically find that $\Lambda_c \approx 0.539$, see the inset in figure 3.

This transition from delocalization to self-trapping in these systems has been predicted and found, both within exact [4, 11–16] and from mean-field calculations [5–7, 10]. To highlight the similarities and discrepancies with the results of this and of the next section, we now briefly review the mean-field approximation. We follow closely the discussion and results of [10]. Mean field may be achieved by first setting the creation and annihilation operators as $c$-numbers, $b_1 \rightarrow b_1^\ast$ and $b_1 \rightarrow b_1$, and further $b_i = |b_i| \exp(i\theta_i)$. Then, one may identify the relative population $p = (|b_1|^2 - |b_2|^2)/N$ and the phase difference $\varphi = \theta_2 - \theta_1$ as classical canonical conjugate variables. Their full dynamics is then determined by the corresponding Hamiltonian (1) in those variables [8, 10, 17].

The ensuing mean-field phase diagram is strikingly similar to the one shown in figure 3, see figure 1 in [10]. It is found that for each value of $\Lambda$, there are just two stationary states that resemble those of $\varepsilon_0(\Lambda)$ and $\varepsilon_N(\Lambda)$ in figure 3, with the mean-field critical interaction being $\Lambda_c^{\text{MF}} = 1/2$. To be precise, for $\Lambda < \Lambda_c^{\text{MF}}$, the energies of the stationary states are $\varepsilon_U(\Lambda) = (\Lambda - 1)/2$ and $\varepsilon_L(\Lambda) = (\Lambda + 1)/2$. For the values $\Lambda \geq \Lambda_c^{\text{MF}}$, there are three stationary states, $\varepsilon_L(\Lambda)$, $\varepsilon_U(\Lambda)$ and $\varepsilon_D(\Lambda) = \Lambda + 1/8\Lambda$. The function $\varepsilon_D(\Lambda)$, for all values of $\Lambda$, essentially coincides with the function $\varepsilon_U(\Lambda)$, the lowest eigenenergy shown as the lower (blue) solid line in figure 3. For $\Lambda < \Lambda_c^{\text{MF}}$, the highest eigenvalue $\varepsilon_U(\Lambda)$ coincides with $\varepsilon_U(\Lambda)$, while for $\Lambda \geq \Lambda_c^{\text{MF}}$, the eigenvalue $\varepsilon_U(\Lambda)$ now approximates to $\varepsilon_U(\Lambda)$. In this region, $\varepsilon_U(\Lambda)$ corresponds to the transition (red) dotted line in figure 3, but in the mean field it turns out to be an unstable solution [5, 8]. There are no further mean-field stationary states within those bounds. That is, all mean-field states within those bounds are non-stationary. This is one of the main differences between the mean field and the exact solution; that is, while all the states bounded by the (blue) solid lines in figure 3 are non-stationary for the mean-field approach, they represent stationary states in the exact quantum calculation.

The mean-field non-stationary states are so because the population $p(\tau)$ shows coherent oscillations for any allowed initial condition and for any allowed value of the mean-field (conserved) energy $\varepsilon$. Those states certainly show the transition from delocalization to self-trapping but in the following way. For $\Lambda < \Lambda_c^{\text{MF}}$ and for a given value of the allowed energies $\varepsilon$, the population $p(\tau)$ oscillates between the boundary values $\pm p_\ast(\varepsilon)$ determined by the energy. Thus, a time average yields $\bar{p}(\tau) = 0$, giving rise to a mean population in well 1 as $N_1 = N(1 + p_\ast(\varepsilon))/2 = N/2$, that is to say, a delocalized state. For the interactions $\Lambda \geq \Lambda_c^{\text{MF}}$ and for the energies $\varepsilon_L < \varepsilon < \varepsilon_U$, again, the time average yields $\bar{p}(\tau) = 0$, $N_1 = N/2$, a delocalized state. However, for energies $\varepsilon_L \leq \varepsilon \leq \varepsilon_D$, the time average may be accurately approximated by $\bar{p}(\tau) \approx p_\ast(\varepsilon)(1 + \sqrt{1 - 1/k^2})/2$, yielding $N_1 \neq N/2$ a self-trapped state. The values of $p_\ast$ and $k^2$ are given by [7, 10]

$$p_\ast = \frac{1}{2\lambda^2}(2\lambda(2\varepsilon - \lambda) - 1 + \sqrt{4\lambda^2 + 1 - 4\lambda(2\varepsilon - \lambda)}),$$

(6)

$$k^2 = \frac{1}{2}\left(1 + \frac{2\lambda(2\varepsilon - \lambda) - 1}{\sqrt{4\lambda^2 + 1 - 4\lambda(2\varepsilon - \lambda)}}\right).$$

(7)

In figure 4 we show a comparison of mean-field versus eigenstate populations, $N_1$ and $\langle N_1 \rangle$, for $\Lambda = 10$, as a function of the energy. We find that while the transition energy $\varepsilon_c(\Lambda)$ agrees well quantitatively for both cases, there is a clear discrepancy for the population values in the self-trapped regime. Note also that the transition in the mean field appears discontinuous. In the next section, we shall analyse the quantum dynamics of coherent states and find that while the period of the oscillations agrees fairly well with their mean-field counterparts, the expectation values of one- and two-body properties in the coherent states decay or collapse to stationary values that agree with those of the quantum eigenstates.

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\[ p(\theta, \phi) = \exp(-i\hat{H}_|/\hbar)\langle \theta, \phi | \hat{N}_1 | \theta, \phi \rangle, \]
and calculate the expectation values of \( \hat{N}_1 \) and \( \hat{c} \):

\[ \langle \hat{N}_1(t) \rangle_c = \langle \theta, \phi | \hat{N}_1 | \theta, \phi \rangle t \]
and

\[ \langle \hat{c}(t) \rangle_c = \langle \theta, \phi | \hat{c} | \theta, \phi \rangle t. \]

As mentioned in the introduction, the coherent state initially with the \( N \) particles in well 1 is given by \( \theta = \pi \) and \( \phi = 0 \). This state has been extensively studied \([4-8, 10-17]\). Here, we shall study all possible coherent states with \( \phi = 0 \). It can then be shown that by varying the angle \( \theta \) from \( \pi/2 \) to a maximum allowed value \( \theta_{\text{max}}(\Lambda) \), the energy \( \epsilon(\theta,0) \) almost span the whole range of energies from \( \epsilon_0(\Lambda) \) to \( \epsilon_N(\Lambda) \), namely \( \epsilon(\pi/2, 0) \lesssim \epsilon_0(\Lambda) \) and \( \epsilon(\theta_{\text{max}}, 0) \lesssim \epsilon_N(\Lambda) \). If \( \theta \) is increased beyond \( \theta_{\text{max}}(\Lambda) \) or reduced below \( \pi/2 \), the energy remains in the same interval \( \epsilon(\pi/2, 0) \approx \epsilon(\theta, 0) \approx \epsilon(\theta_{\text{max}}, 0) \). However, the expectation value of the number of particles \( \langle \hat{N}_1(t) \rangle_c \) does register this change, as we discuss below.

Figures 5 and 7 show the time evolution of the expectation values \( \langle \hat{N}_1(t) \rangle_c \) and \( \langle \hat{c}(t) \rangle_c \), in the three arbitrary initial coherent states, see the figure captions, and for three typical values of \( \Lambda \). Figure 6 shows the comparison of \( \langle \hat{N}_1(t) \rangle_c \) with the corresponding mean-field calculations. The latter are obtained by setting the energy of the mean-field solution equal to the expectation value of the energy in the coherent state, namely \( \epsilon = \epsilon(\theta, 0) \) for the given value of \( \Lambda \).

For the case \( \Lambda = 0.1 \), the first panels of figures 5 and 6, the system shows coherent oscillations initially, then it falls into a stationary value with \( \langle \hat{N}_1(t) \rangle_c = N/2 \) within numerical accuracy, followed by revivals at almost periodic intervals. The stationary value agrees with the mean-field time average, as shown in figure 6.

For \( \Lambda = 1.0 \), second panels of figures 5 and 6, the system is already in the self-trapped regime for the chosen initial condition. The mean-field counterpart does show coherent oscillations and their time average, for this value of \( \Lambda \), agrees fairly well with the stationary value of the fully quantum evolved state.

At \( \Lambda = 10.0 \), third panels of figures 5 and 6, the system is well into the self-trapped regime and there again appear regions of coherent oscillations followed by stationary intervals in the full quantum evolution, while the mean-field calculation oscillates around an average value close but different from the stationary value.

We observe that the behaviour of the two-body correlation \( \langle \hat{c}(t) \rangle_c \), in figure 7 follows essentially the same pattern of stationary collapsed regions followed by revivals, as the population \( \langle \hat{N}_1(t) \rangle_c \), in figure 5.

The point that we stress here is the fact, numerically verified, that the time spent in the stationary regions becomes longer than the time spent in the coherent-oscillation sections, as the number of particles \( N \) increases. One finds, generally,

\[ \langle \theta, \phi \rangle = \sum_{n_1=0}^{N} \binom{N}{n_1}^{1/2} \sin^{N-n_1}(\theta/2) \times \cos^{n_1}(\theta/2) e^{-i(N-n_1)\phi} |n_1, N-n_1 \rangle \]
that the time between recurrences scales as \( \tau_r = A(\Lambda)N^\alpha \)
while the time during the recurrence, that is, the relaxation time, scales as \( \tau_d = B(\Lambda)N^\gamma \). The coefficients \( A \) and \( B \) are \( \Lambda \)-dependent, but the exponents appear to be quite universal taking the values \( \alpha \approx 1 \) and \( \gamma \approx 0.5 \). It is worth to mention that for the initial condition \( |N, 0 \rangle \) analytical expressions for the collapse and revival times may be found \[11\] that are in agreement with our general observation for all values of \( \Lambda \). We can therefore conclude that the ratio \( \tau_d/\tau_r \to 0 \) as \( N \to \infty \). This is in marked contrast to the mean-field behaviour. We believe that this is a very important point. That is, based on the facts that macroscopically and experimentally we are very much limited to access physical properties of few bodies only, such as energies, temperatures and correlations functions, thus, measurements of, say, \( \hat{N}_1 \) and \( \hat{C} \) at different times, starting each realization in the same state, necessarily yield the conclusion that the system is, within fluctuations, around a mean stationary value. We call these statistically stationary states to distinguish them from the true stationary energy eigenstates.

Once we have shown that the system reaches statistically stationary states, we can describe their properties by the given values of the mean of \( \langle \hat{N}_1(t) \rangle_c \) and \( \langle \hat{C}(t) \rangle_c \), namely by their statistically stationary values denoted as \( N_1^c \) and \( C^c \). This family is built in the following manner. For given values of \( N \) and \( \Lambda \), and taking \( \phi = 0 \), we find the values of \( \theta \) such that the expectation values of the energy in the coherent states span the whole interval \( \epsilon_0(\Lambda) \leq \epsilon(\theta, 0) \leq \epsilon_N(\Lambda) \). Then, we evaluate the time evolution of the corresponding coherent state \( |\theta, 0, t \rangle \) and calculate \( N_1^c \) and \( C^c \). Clearly, the value of \( \theta \) for a given energy is not unique. We see below that, depending on the value of \( \theta \), the coherent state can break the symmetry. If it does, it localizes either near well 1 or well 2, once the condition for self-trapping is satisfied, i.e. for \( \Lambda \geq \Lambda_c \).

Figure 5. Time evolution of the expectation value of the number of particles in well 1, \( \langle \hat{N}_1 \rangle_c \), in the coherent states \( \phi = 0 \), and \( \theta = \pi + 0.1 \) for \( \Lambda = 0.1 \), \( \theta = \pi + 0.1 \) for \( \Lambda = 1.0 \), and \( \theta = \pi - 1.0 \), for \( N = 1000 \).

Figure 6. Comparison of the mean-field (blue) solid line versus the full quantum evolution (red) dotted line of the time evolution of the expectation value of the number of particles in well 1, \( \hat{N}_1(t)/N \), both having the same energy. The coherent states are \( \phi = 0 \), \( N = 1000 \), and \( \theta = \pi + 0.1 \) for \( \Lambda = 0.1 \), \( \theta = \pi + 0.1 \) for \( \Lambda = 1.0 \), and \( \theta = \pi - 1.0 \) for \( \Lambda = 10.0 \). The corresponding energies are \( \epsilon = 0.15, 1.04 \) and 6.03, respectively.

Figure 7. Time evolution of the expectation value of the tunnelling correlation, \( \langle \hat{C} \rangle_c \), in the coherent states \( \phi = 0 \), \( N = 1000 \), and \( \theta = \pi + 0.1 \) for \( \Lambda = 0.1 \), \( \theta = \pi + 0.1 \) for \( \Lambda = 1.0 \), and \( \theta = \pi - 1.0 \) for \( \Lambda = 10.0 \).
Figure 8. Statistically stationary value of the number of particles in well 1, \( N_1' \), in the family of coherent states \( |\theta, 0; t\rangle \), as a function of their expectation value of the energy \( \varepsilon(\theta, 0) \), for \( N = 1000 \), the (red) solid line. For comparison, in the (blue) dotted line the corresponding expectation values in the energy eigenstates \( \langle \hat{N}_1 \rangle \) (same as in figure 1). In the second panel, we show the statistically stationary states localized in well 1, while in the third panel, the statistically stationary states localized in well 2. See the text.

Figure 9. Statistically stationary value of the tunnelling correlation, \( \tilde{C} \), in the family of coherent states \( |\theta, 0; t\rangle \), as a function of their expectation value of the energy \( \varepsilon(\theta, 0) \), for \( N = 1000 \), the (red) solid line. For comparison, in the (blue) dotted line the corresponding expectation values in the energy eigenstates \( \langle \hat{C} \rangle \) (same as in figure 2).

Figures 7 and 8 show the stationary values \( N_1' \) and \( \tilde{C} \) for \( N = 1000 \) and for \( \Lambda = 0.1, 1.0 \) and 10.0 as a function of the expectation value of the energy of the state. In the same graph we have included the eigenstate expectation values of figures 1 and 2. In general, we see that the stationary values from the coherent states \( N_1' \) and \( \tilde{C} \) agree fairly well with the corresponding eigenstate values. Hence, we can conclude that the macroscopic behaviour of the statistically stationary states is also described by the phase diagram shown in figure 3, since they behave similarly to the energy eigenstates. That is, there exists a critical value \( \Lambda_c \), such that for values above such a threshold the system exhibits a self-trapping transition as a function of the energy (or as a function of the initial state). Additionally, the states may be well characterized by both one- and two-body properties; that is, while the one-body properties remain constant below the self-trapping transition, two-body variables serve to discriminate among different states. Both quantities clearly signal the transition point. As an additional aspect, note in figures 8 and 9 that the transition appears continuous for the statistically stationary states. However, one can again speculate that as \( N \) increases the transition may remain continuous but probably with a discontinuous derivative.

The transition from delocalized to self-trapped states exhibits a symmetry-breaking phenomenon. That is, the Hamiltonian is symmetric under the exchange of the wells, or internal states, 1 and 2. However, the stationary states ‘choose’ one of the wells to become localized. To be precise, one can show that for \( \Lambda \geq \Lambda_c \), if \( \phi = 0 \) and \( \theta \) yields a state localized in well 1, then \( \theta' = \pi - \theta \) and \( \phi = 0 \) localize in well 2. This is illustrated in figure 8: for \( \Lambda = 1.0 \) the (red) solid line signals localization in well 1 and for \( \Lambda = 10.0 \) the (red) solid line localizes in well 2.

4. Final remarks

We have analysed one- and two-body properties of the full quantum solution of the two-mode Bose–Hubbard fluid. We have discussed the transition from delocalized to self-trapped states, which occurs as the energy of the system is increased, provided that the pair-interaction strength is above a critical or threshold value. The full quantum solution for a large number of atoms differs from the mean-field approximation, since the latter predicts coherent Josephson-like oscillations while the exact solution shows that these oscillations decay to stationary-like states in which the system spends most of its time. Since, measuring or having access to the \( N \)-body wavefunction appears as an impractical task in real systems, most of our understanding of macroscopic systems is based on knowledge of properties of few bodies. In this context, we argue that the decay, or relaxation, to a stationary state can be considered as decoherence [23], even if no interaction with an external environment is included. Such a decoherence is a consequence of the interatomic interactions.

Taking the statistical description of the stationary states as an approach to characterize them, we have studied the number of particles in well 1 \( \hat{N}_1 \) and the tunnelling correlation \( \tilde{C} \), see equations (4) and (5), as examples of one- and two-body
properties. The phase diagram of figure 3 summarizes our results. For given values of the number of particles $N$ and the interaction strength $\Lambda$, we find a transition from delocalized to self-trapped states as a function of the energy $\varepsilon$ of the fluid, if $\Lambda \gtrsim \Lambda_c$, a critical interaction value. One finds that $N_1$ remains constant, $N_1 = N/2$, up to a critical energy value $\varepsilon_c(\Lambda)$, where it changes up to either a value $N_1 \approx 0$ or $N_1 \approx N$, as the energy is further increased. Likewise, the transition is registered by $C$ with a cusp at the transition energy, clearly dividing two different types of macroscopic states.

The delocalization to self-trapping transition, within our calculations, appears to be a discontinuous one in the behaviour of $\langle \hat{N}_1 \rangle$ in the eigenstates while continuous in $\langle \hat{C} \rangle$, with a clear symmetry-breaking mechanism. That is, while the Hamiltonian is invariant under the interchange of ‘1’ and ‘2’ of the wells, statistically stationary and eigenstates with the same energy are not. A set of states localizes in well 1 and another in well 2. On the other hand, as mentioned already, there is evidence both from the coherent states and from the analysis of larger values of $N$ that the transition may become continuous but sharp, in the sense that the derivatives may become discontinuous. All this evidence indicates that $N_1$ behaves as the order parameter of the transition [27] in a way analogous to the behaviour of the magnetization of a ferromagnetic material [28]. This aspect of the transition certainly deserves further research.

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