A heuristic approach to BEC self-trapping in double wells beyond the mean field

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Received 20 December 2011, in final form 10 February 2012
Published 26 March 2012
Online at stacks.iop.org/JPhysB/45/085303

Abstract
We present a technically simple treatment of self-trapping of Bose–Einstein condensates in
double well traps based on intuitive semiclassical approximations. Our analysis finally leads to
a convenient closed-form approximation for the time-averaged population imbalance valid in
both the mean-field case and in the case of finite particle numbers for short times.

((Some figures may appear in colour only in the online journal)

1. Introduction

Despite its simplicity, an atomic Bose–Einstein condensate (BEC) in a double well trap is a quantum system showing a
rich dynamical behaviour in different parameter ranges that can be quite accurately controlled in current experiments (see
e.g. [1–3] and references therein). Even in the mean-field limit
of high particle numbers \( N \), where many-particle correlations
are neglected, different dynamical regimes are observed. The latter can be understood by mapping the system to a
classical pendulum the dynamics of which can be analysed in
the corresponding two-dimensional phase space (see e.g. [4]).
For small and moderate interaction \( U \) between the particles,
a condensate that is initially localized in one of the two wells
performs Rabi respectively Josephson oscillations between the
two wells. If the inter-particle interaction exceeds a critical
value, the initially occupied well remains macroscopically
occupied due to spontaneous symmetry breaking. This is
referred to as the running phase self-trapping effect.

While for finite particle numbers the self-trapping effect is eventually destroyed by quantum correlations in the long-
time limit, it can still be observed for a considerable time span depending on the number of particles in the system
[5, 6]. In this ‘short-time regime’ the main dynamical features of the system are well described by (semi-) classical phase
space methods like the truncated Wigner approximation [7] or a similar ansatz based on the Husimi distribution
[8–10], where the respective quantum-mechanical phase space representations of an initial quantum state are sampled by an
ensemble of trajectories that are propagated according to the
corresponding Gross–Pitaevskii mean-field equation. Related
aspects of the system studied in the literature include the
semiclassical WKB-type quantization of its energy spectrum
[11] and the quantum fluctuations of the eigenstates near the
point of transition to self-trapping [12].

In this paper, following the example of [13, 14],
the transition to self-trapping is described by means of a single scalar quantity, namely the time average \( \bar{z}(\Lambda) \) of the relative
population imbalance between the two wells as a function of the
scaled interaction parameter \( \Lambda = U(N-1)/J \), where \( J \) is the tunnelling coefficient (cf equation (1) below). It will be
shown that a useful closed-form approximation for \( \bar{z}(\Lambda) \) in
the aforementioned semiclassical parameter and time regimes
can be derived in a technically simple manner by means of
intuitive heuristic approximations.

This paper is organized as follows. In section 2, we discuss
some selected properties of the system Hamiltonian, namely the Bose–Hubbard dimer and its mean-field limit. In section 3,
we use a heuristic ansatz to derive a closed-form approximation for the time-averaged population imbalance as a function of the
scaled interaction strength for the mean-field case. In section 4,
many-particle effects are taken into account in a semiclassical
manner by incorporating quantum fluctuations of the initial
state into the mean-field description derived in the previous
section which again leads to a closed-form approximation for
the time-averaged population imbalance. The main results are
briefly summarized in section 5. The appendix contains a brief
review of the dynamics of the corresponding noninteracting system.
2. The Hamiltonian

For low energetic excitations and low temperatures, it is possible to consider only the local ground states of the left and right wells and neglect all energetically higher states of the double well trap. In this two-mode approximation, the double well system is described by the Bose–Hubbard dimer Hamiltonian (cf. e.g. [3])

\[
\hat{H} = -\frac{J}{2}(\hat{a}_L^\dagger \hat{a}_R^\dagger \hat{a}_R + \hat{a}_L^\dagger \hat{a}_L) + \frac{U}{2}(\hat{a}_L^\dagger)^2 \hat{a}_L^2 + (\hat{a}_R^\dagger)^2 \hat{a}_R^2 \\
+ \epsilon_L \hat{a}_L^\dagger \hat{a}_L + \epsilon_R \hat{a}_R^\dagger \hat{a}_R,
\]

where \( \hat{a}_L \) and \( \hat{a}_R \) are the annihilation operators of a particle in the left and right wells, respectively. The quantities \( J \) and \( U \) depend on the shapes of the local ground states in the two wells. \( J > 0 \) determines the rate of tunnelling between adjacent lattice sites, \( U \) is the inter particle interaction parameter and \( \epsilon_L, \epsilon_R \) are the on-site energy terms. Here, we concentrate on repulsive interaction \( U > 0 \).

For a sufficiently high number of particles \( N \) in the system, one can apply a Hartree–Fock mean-field approximation (see e.g. [15]) where the operators \( \hat{a}_L, \hat{a}_R \) in the Hamiltonian can be replaced by the complex numbers \( \sqrt{N}/\sqrt{L} \) representing their respective coherent state expectation values. This leads to the ‘classical’ Hamiltonian

\[
H/N = -\frac{J}{2}(c_L^\dagger c_R + c_R^\dagger c_L) + \frac{U}{2}(|c_L|^4 + |c_R|^4) \\
+ \epsilon_L |c_L|^2 + \epsilon_R |c_R|^2.
\]

The canonical equations of motion \( i\hbar \dot{c}_L = i\hbar \dot{c}_R = 0 \), \( i\hbar c_L = \sin \theta (\hat{a}_L + \hat{a}_R) \) then lead to the coupled discrete Gross–Pitaevskii equations or nonlinear Schrödinger equations

\[
i\hbar \dot{c}_L = -\frac{J}{2}c_R + (\epsilon_L + U(N - 1)|c_L|^2)c_L,
\]

\[
i\hbar \dot{c}_R = -\frac{J}{2}c_L + (\epsilon_R + U(N - 1)|c_R|^2)c_R,
\]

which describe the mean-field dynamics of the on-site amplitudes. Particle number conservation yields \( |c_L|^2 + |c_R|^2 = 1 \).

Introducing the amplitude-phase representation \( c_R = \sqrt{\rho} \exp(i\theta_R), c_L = \sqrt{1 - \rho} \exp(i\theta_L) \), the classical Hamiltonian (2) reads

\[
H/N = -J\sqrt{(1 - \rho)} \cos \theta + \frac{U}{2}(N - 1)((1 - \rho)^2 + \rho^2) \\
+ \epsilon_L (1 - \rho) + \epsilon_R \rho,
\]

with \( \theta = \theta_R - \theta_L \).

In the following we consider the situation of a symmetric double well where \( \epsilon_L = 0 = \epsilon_R \) and initial conditions where all particles occupy the left site, i.e. \( |c_L|^2 = 1 \), \( |c_R|^2 = 0 \) respectively \( \rho = 0 \) at time \( t = 0 \). Then the corresponding conserved energy per particle reads \( E/N = H(p = 0)/N = U(N - 1)/2 \). We assume that self-trapping occurs if an equal population of both sites, i.e. \( |c_L|^2 = 1/2 = |c_R|^2 \) respectively \( \rho = 1/2 \) is no longer possible. Conservation of energy yields (cf. e.g. [4]) \( E/N = H(p = 1/2)/N \) which leads to the condition \( \cos \theta = U(N - 1)/(2J) \). \( |\cos \theta| \leq 1 \) implies that an equal occupation of both sites is only possible for \( |U(N - 1)/J| \leq 2 \) so that self-trapping occurs if

\[
\Lambda = \frac{U(N - 1)}{J} > 2
\]

(for \( U > 0, J > 0 \)). Please note that the effect considered here is referred to as running phase self-trapping and should not be confused with so-called \( \pi \)-phase self-trapping that is closely related to the appearance of symmetry breaking nonlinear eigenstates of the Gross–Pitaevskii equations (3), (4) (see e.g. [4, 16] for a more detailed discussion).

3. Heuristic mean-field approach

In the mean-field case, described by the Hamiltonian (2) and the corresponding Gross–Pitaevskii equations (3), (4), the site populations \( |c_L|^2 \) and \( |c_R|^2 \) are periodic in time [4]. In the following, we can thus quantify the self-trapping by means of the time-averaged relative population imbalance (cf. [13, 14])

\[
\bar{\rho} = |c_L|^2 - |c_R|^2 = 1 - 2\bar{p} \quad -1 \leq \bar{\rho} \leq 1,
\]

where the overbar denotes time-averaged quantities and \( p = \rho \) as introduced in the previous section. For the mean-field Gross–Pitaevskii case, an exact solution in terms of elliptic integrals was derived in [13]. Here, we instead aim at a convenient approximation in terms of elementary functions.

To this end, we first consider the noninteracting limit of our system, as described by equations (3), (4) with \( U = 0 \). If at time \( t = 0 \), all particles are in the left well, the occupation \( |c_L(t)|^2 \) is equal to \( |c_L|^2 \) as introduced in the previous section. For the mean-field Gross–Pitaevskii case, an exact solution in terms of elliptic integrals was derived in [13]. Here, we instead aim at a convenient approximation in terms of elementary functions.

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In the interacting case with a finite \( U > 0 \), the time-dependent local chemical potentials of the two sites read \( \epsilon_L + U(N - 1)|c_L|^2 \) and \( \epsilon_R + U(N - 1)|c_L|^2 \), respectively (cf. (3), (4)). We therefore introduce the interaction into (8) in a heuristic manner by replacing \( \Delta \) with the time-averaged difference of the on-site terms, i.e. we set \( \Delta = \epsilon_L - \epsilon_R + U(N - 1)(|c_L|^2 - |c_R|^2) = \epsilon_L - \epsilon_R + JA(1 - 2\bar{p}) \). For the special case of a symmetric double well where \( \epsilon_L = 0 = \epsilon_R \), equation (8) thus becomes

\[
p(t) = \frac{1}{1 + \Lambda^2(1 - 2\bar{p})^2} \sin^2 \left( \sqrt{1 + \Lambda^2(1 - 2\bar{p})^2} \frac{J}{2\hbar} t \right).
\]

Self-consistency then requires

\[
\bar{p} = \frac{1}{2} - \frac{1}{1 + \Lambda^2(1 - 2\bar{p})^2},
\]

where we have inserted the time average \( \sin \bar{\rho} t = 1/2 \). It is convenient to replace \( \bar{\rho} \) by \( \bar{\rho} \) via (7),

\[
\bar{\rho} = 1 - \frac{1}{1 + \Lambda^2 \bar{\rho}^2},
\]

which yields the cubic equation

\[
\bar{\rho}^3 - \bar{\rho} + \frac{1}{\Lambda^2} \bar{\rho} = 0.
\]
that oscillation observed in the mean-field case and the low
finite number fluctuations. Heuristic semiclassical ansatz: adding quantum
For the scaled interaction strength $\Lambda = U(N-1)/J$ compared to the
approximation (13) (-).
the noninteracting case (3), (4). Gross–Pitaevskii equations (3), (4).
numerically exact mean-field values obtained by integrating the
Gross–Pitaevskii equations (3), (4). Considering the
simplicity of our approach, we observe good agreement between the curves. The deviations for $\Lambda \gtrsim 2$ are mainly due to the fact that the ansatz does not take into account the
change in the shape of the oscillations from sinusoidal to Jacobi
elliptic caused by the nonlinearity (cf [4]).

4. Heuristic semiclassical ansatz: adding quantum fluctuations
In this section, we consider the Bose–Hubbard dimer (1) with
a finite number $N$ of particles. In [5, 6], the dynamics of the
initial state $|N, 0\rangle$, i.e. the number state where all particles
are in the left well, was analysed in the regime of strong interaction by treating the tunnelling terms proportional to $J$ as a small perturbation which yields the time-dependent population imbalance
$$z(t) = \left[ 1 - \frac{(J/U)^2(N/2 + 1)}{2(N - 1)^2} \cos(\omega_{0t}) \right] \cos(\omega_{0t})$$
$$+ \frac{(J/U)^2(N/2 - 1)}{2(N - 1)^2} \cos(\omega_{0t})$$
$$+ \frac{(J/U)^2}{(N - 1)^2} \cos(\omega_{0t}/2) \cos(\omega_{0t}) + O((U/J)^3) \quad (14)$$
with the high frequency $\omega_{0t} = U(N-1)/h - J^2(N+1)/[2U(N^2 - 4N + 3)]$ that corresponds to the Josephson oscillation observed in the mean-field case and the low
frequencies $\omega_1 = U(N-1)(N-2)/(2N-3)(N-3!)$ and $\omega_0 = U(N_1)/[2(N-1)!]$ which quickly decrease with the number of particles in the system. Thus, even for moderately high particle numbers, these low frequencies only become relevant for times that are long compared to the
Josephson tunnelling time $\pi/J$.

This means that the self-trapping effect is destroyed by quantum correlations in the long-time limit when the oscillation with frequency $\omega_0$ leads to a total population transfer between the two sites. Nevertheless, self-trapping can be observed for a considerable time span given by the condition $\omega_{0t} \ll 1$. The short-time regime, which we will consider in the
following, is further characterized by the condition $\omega_{0t} \ll 1$.
In this limit the population imbalance (14) becomes [6]
$$z(t) = \left[ 1 + (J/U)^2/2(N-1)^2 \right] \cos(\omega_{0t}) - 1 + O(U/J)^3$$
which yields the time average $\bar{z} = 1 - (J/U)^2/2(N - 1)^2 + O((U/J)^3) = 1 - 1/(2\Lambda^2) + O((U/J)^3)$. Thus, the perturbative approach is unable to describe the system’s behaviour in the vicinity of the self-trapping transition point.
For moderate interaction strengths, where the perturbative treatment of the tunneling terms is not a good approximation, the self-trapping effect can still be observed for a time span much longer than the Josephson tunnelling time before it is
destroyed. This is illustrated in figure 2 which shows the time-
dependent population imbalance $z(t)$ for $N = 100$ and $\Lambda = 2$
for the initial state $|N, 0\rangle$. The time is given in multiples of
$\tau_0 = 2\pi/\omega_0$ where $\omega_0 = J/h$ is the Rabi frequency in the
noninteracting case $U = 0$ (cf appendix). For shorter times, the
system shows self-trapping similar to the mean-field case (left panel). For longer times an oscillation with a higher amplitude and a longer period is revealed (right panel). For even longer times, which are beyond the range of numerical accuracy for the
given parameters, the self-trapping effect is expected to be
completely destroyed as in the weak tunnelling limit discussed above (cf discussion in [5, 6]).

In the short time regime, the dynamics of the system is quite well described by semiclassical phase space methods
where quantum mechanical phase representations of the
initial quantum state like the Wigner [7] or Husimi [8–10]
distributions are propagated in phase space according to the
Gross–Pitaevskii equations (3), (4).
In the spirit of these semiclassical methods, we want to add the quantum fluctuations of the initial state to the simple
mean-field description developed in the previous section. Since expression (11) for the time-averaged relative population imbalance only depends explicitly on the amplitude of the oscillation (and thus on the local particle numbers in the wells) but not on the relative phase between the wells, we want to incorporate the quantum fluctuations of the initial state via the fluctuations of the local particle numbers. To estimate the particle number fluctuations, we consider the approximate
mean-field dynamics of the relative particle number in the right
well given in (9), which can be conveniently rewritten as
$$p(t) = p_{\text{amp}} \sin^2(\omega_{\Lambda} t) \quad (15)$$
with the abbreviations $p_{\text{amp}} = (1 + \Lambda^2(1 - 2\tilde{\rho})^2)^{-1}$ and
$\omega_{\Lambda} = \sqrt{1 + \Lambda^2(1 - 2\tilde{\rho})^2}/(2\Lambda)$. For interaction strengths
$\Lambda \gtrsim 2$ near the transition point, where we expect the quantum
fluctuations to have their greatest influence, the model (13) predicts $\tilde{z} \approx 1/2$ which implies $p \approx 1/4$ and $p_{\text{amp}} \approx 1/2$, i.e. half of the particles take part in the oscillation.

Particle number fluctuations of mean-field like states were recently analysed in [18]. Following [18], we define the operators

$$\hat{a}_0 = \sqrt{1-p}\hat{a}_L + \sqrt{p}\exp(i\theta)\hat{a}_R,$$

$$\hat{a}_L = -\sqrt{p}\exp(i\theta)\hat{a}_L + \sqrt{1-p}\hat{a}_R,$$  \hspace{1cm} (16)

where $\hat{a}_0$ destroys a state with occupations $1-p$ in the left well and $p$ in the right well respectively with a relative phase $\theta$, and $\hat{a}_L$ destroys a state orthogonal to the first one. A mean-field-like state with $N$ particles and occupations $1-p$ in the left and $p$ in the right is thus given by

$$|\psi_0\rangle = (N!)^{-1/2}(\hat{a}_0^\dagger)^N|0\rangle.$$  \hspace{1cm} (17)

The inversion of relation (16) reads

$$\hat{a}_R = \sqrt{p}\exp(i\theta)\hat{a}_0 + \sqrt{1-p}\hat{a}_L,$$

$$\hat{a}_L = \sqrt{1-p}\hat{a}_0 - \sqrt{p}\exp(i\theta)\hat{a}_L.$$  \hspace{1cm} (18)

The fluctuations of the particle number $\hat{n}_R = \hat{a}_R^\dagger\hat{a}_R$ in the right well are given by $\Delta\hat{n}_R = \langle \psi_0 | \hat{a}_R^\dagger \hat{a}_R | \psi_0 \rangle - \langle \psi_0 | \hat{a}_R | \psi_0 \rangle^2$. Using (18) $\hat{n}_R$ can be expressed in terms of $\hat{a}_0$ and $\hat{a}_L$ so that the expectation values with respect to $|\psi_0\rangle$ can be evaluated in a straightforward manner which yields (cf [18])

$$\Delta\hat{n}_R = N(p(1-p)).$$  \hspace{1cm} (19)

For an initial state with $p=0$ (i.e. all particles in the left well), the particle number fluctuations vanish and there are only phase fluctuations which cannot be incorporated easily into our classical model (13) whereas it is quite straightforward, as shall be shown in the following, to include number fluctuations. Since the approximate mean-field dynamics (15) is periodic (as is the exact one, see e.g. [4]), each mean-field state at some time $t \in [0, \pi/\omega_\Lambda]$ creates the same dynamics (apart from an irrelevant phase shift) if chosen as the initial state. For practical reasons, we can thus choose an initial state whose quantum fluctuations are dominated by number fluctuations rather than phase fluctuations. We therefore consider the state at $t = \pi/(2\omega_\Lambda)$ as an initial state where $p = p_{\text{amp}}$ and particularly $p_{\text{amp}} = 1/2$ for $\Lambda = 2$. For this state the particle number fluctuations (19) assume their maximum $\Delta\hat{n}_R^2 = N p_{\text{amp}}(1-p_{\text{amp}}) = N/4$. This corresponds to a standard deviation of the amplitude $p_{\text{amp}} = \langle \hat{n}_R \rangle/N$ of $\text{std}(p_{\text{amp}}) = \Delta\hat{n}_R^2/N = 1/(2\sqrt{N})$. The standard deviation of the time-averaged population imbalance $\tilde{z}$ is then given by

$$\text{std}(\tilde{z}) = 2\text{std}(p_{\text{amp}})\sin^2(\omega_\Lambda t) = \frac{1}{2\sqrt{N}}.$$  \hspace{1cm} (20)

Please note that these fluctuations, in accordance with the truncated Wigner and Husimi methods, correspond to the fluctuations of the initial state only and do not represent the actual time average of the quantum fluctuations. Applying the central limit theorem, we assume the fluctuations to be Gaussian for the particle numbers $N \geq 50$ considered in the following.

Now the initial quantum fluctuations can be added to our classical description by means of the replacement $\tilde{z} \rightarrow \tilde{z} + \delta\tilde{z}$ on the right-hand side of (11),

$$\tilde{z} = 1 - \frac{1}{1 + \Lambda^2(\tilde{z} + \delta\tilde{z})^2},$$  \hspace{1cm} (21)

where $\delta\tilde{z}$ is a Gaussian random variable with zero mean and standard deviation (20). To lowest order in $\delta\tilde{z}$, we obtain the cubic equation

$$\tilde{z}^3 + (2\delta\tilde{z} - 1)\tilde{z}^2 + \left(\frac{1}{\Lambda^2} - 2\delta\tilde{z}\right)\tilde{z} = 0$$  \hspace{1cm} (22)

which yields, in analogy with (13),

$$\tilde{z}(\Lambda, \delta\tilde{z}) = \begin{cases} 0, & \text{if } \delta\tilde{z} < -1/\Lambda \text{ or } \delta\tilde{z} > 1/\Lambda, \\ \frac{1}{2} - \delta\tilde{z} + \sqrt{\left(\delta\tilde{z} + \frac{1}{2}\right)^2 - \frac{1}{\Lambda^2}}, & \text{if } -1/\Lambda \leq \delta\tilde{z} < 0, \\ \frac{1}{2} + \delta\tilde{z} + \sqrt{\left(\delta\tilde{z} - \frac{1}{2}\right)^2 - \frac{1}{\Lambda^2}}, & \text{if } 0 < \delta\tilde{z} < 1/\Lambda. \end{cases}$$  \hspace{1cm} (23)

The semiclassical result for the time-averaged relative population imbalance can thus be directly obtained by averaging over (23) with $\delta\tilde{z} = \zeta/(2\sqrt{N})$, where $\zeta$ is a standard Gaussian random variable with mean($\zeta$) = 0 and std($\zeta$) = 1.

Neglecting fluctuations with $\delta\tilde{z} < -1/\Lambda$ or $\delta\tilde{z} > 1/\Lambda$, the time-averaged relative population imbalance can alternatively be expressed as the integral

$$\tilde{z}(\Lambda) = \int_{s_0}^{s_\Lambda} \left(\frac{1}{2} - x + \sqrt{\left(\frac{1}{2} + x\right)^2 - \frac{1}{\Lambda^2}}\right) \frac{\exp\left(-\frac{x^2}{2\sigma_n^2}\right)}{\sqrt{2\pi \sigma_n^2}} \, dx,$$  \hspace{1cm} (24)

$$= \frac{1}{2}\Phi\left(-\frac{x_0}{\sigma_N}\right) - \sigma_N\Phi\left(\frac{x_0}{\sigma_N}\right) + \int_{s_0}^{s_\Lambda} \sqrt{\left(\frac{1}{2} + x\right)^2 - \frac{1}{\Lambda^2}} \frac{1}{\sigma_N} \Phi\left(\frac{x}{\sigma_N}\right) \, dx.$$  \hspace{1cm} (25)
In figure 3, we compare our approximation for $\tilde{\bar{\varepsilon}}(\Lambda)$ with the numerically exact results for different values of the particle number $N$. To obtain the numerically exact short time results, we compute the dynamics of the system in the Fock basis $|n\rangle$, $0 \leq n \leq N$, for the initial state $|N\rangle$ and average over the time interval $[0, 100\sigma]$. Generally, we observe good agreement between the approximation and the numerical results. The small deviations around $\Lambda \approx 2$ that are inherited from the heuristic mean-field approach are related to the influence of the mean-field interaction on the shape of the oscillations. The deviation is less pronounced for smaller particle numbers since the quantum fluctuations lead to deviations from the characteristic shape of the mean-field oscillations (cf figure 2) that are given by Jacobi elliptic functions \cite{4}. The additional deviations observed for $N = 50$ are caused by the fact that for this relatively small particle number some effects of low-frequency modes (cf figure 2 and the discussion at the beginning of the section) can be felt even for short times for interaction strengths around $\Lambda \approx 2$. Qualitatively, our results confirm the behaviour found in a previous numerical study \cite{13}. The quantum fluctuations cause a broadening and softening of the transition region between the Josephson oscillation regime and the self-trapping regime. Quantitatively, however, there are some deviations because in \cite{13} the time averages are performed over much longer time intervals such that the system dynamics is influenced by the low-frequency modes mentioned above.

In the limit $\Lambda \to \infty$ of infinite interaction strength, the particle number $N$ for the threshold value $\alpha = 0.001$.

Since there is no longer a sharp transition point for finite particle numbers $N$, we quantify the shift of the transition point by considering the interaction strength $\Lambda$ for which the population imbalance $\tilde{\bar{\varepsilon}}$ surpasses a certain small threshold value $\alpha$ (cf \cite{13}). This happens in the region where $x^* = x_0 = 1/\Lambda - 1/2$, so that $\tilde{\bar{\varepsilon}}(\Lambda) \approx \Phi((1 - 2/\Lambda)\sqrt{\Lambda})/2$. Setting this expression equal to $\alpha$, we obtain the condition

$$\Lambda_\alpha \approx 2(1 - N^{-1/2}\Phi^{-1}(2\alpha))^{-1}$$  \hspace{0.5cm} (27)

with the inverse function $\Phi^{-1}(x) = \sqrt{2}\text{erf}^{-1}(2x - 1)$ known as a quantile function. For high particle numbers $N \gg 1$, the critical interaction strength behaves like $\Lambda_\alpha \approx 2 + 2\Phi^{-1}(2\alpha)N^{-1/2}$. In the limit $N \to \infty$, one recovers the mean-field result $\Lambda = 2$, which is independent of $\alpha$, indicating a sharp transition point. Figure 4 illustrates the dependence of the critical interaction strength (27) on the particle number $N$ for the threshold value $\alpha = 0.001$, $\Phi^{-1}(2\alpha) \approx -2.8782$.

In this paper, we have described the transition to self-trapping of BECs in double wells by a single scalar quantity, namely the time-averaged relative population imbalance between the wells as a function of the scaled interaction strength. Using a heuristic ansatz we have derived convenient closed-form approximations for the time-averaged relative population imbalance in the two-mode Bose–Hubbard approximation that are valid in the classical (mean field) and semiclassical parameter and time regimes, respectively. The comparison with numerically exact results has revealed good agreement.
Our technically simple treatment thus complements more rigorous numerical studies of the problem based on semiclassical phase space methods as well as exact methods like the numerical diagonalization in Fock space. Unlike other approaches, the present treatment concentrates from the very beginning on the description of symmetry breaking by means of time-averaged quantities, thereby demonstrating that the self-trapping effect is mostly independent of the details of the quantum dynamics, both in the mean-field case and in the case of finite particles for short times.

Due to its simplicity, the Bose–Hubbard dimer considered in this work is an important model for the investigation of symmetry breaking effects in interacting quantum systems. Its usefulness is further supported by the fact that many other systems can be mapped to or approximated by a two-mode system. Yet, one must keep in mind that certain methods which work for the Bose–Hubbard dimer, like e.g. WKB quantization [11], can not be straightforwardly applied to other systems. The present treatment concentrates from the very beginning on the description of symmetry breaking by means of time-averaged quantities, thereby demonstrating that the self-trapping effect is mostly independent of the details of the quantum dynamics, both in the mean-field case and in the case of finite particles for short times.

Appendix. The noninteracting two-mode system

In the noninteracting case the dynamics of the site amplitudes is governed by the linear Schrödinger equations

\[ ih\dot{c}_L = - \frac{J}{2} c_R + \epsilon_L c_L \quad (A.1) \]

\[ ih\dot{c}_R = - \frac{J}{2} c_L + \epsilon_R c_R \quad (A.2) \]

which are readily obtained by setting \( U = 0 \) in the Gross–Pitaevskii equations (3), (4). Inserting the ansatz \( c_R(t) = \exp(i\Omega t) \) and eliminating \( c_L \) yields the characteristic equation \( \hbar^2 \Omega^2 + (\epsilon_L + \epsilon_R)\hbar\Omega + \epsilon_L\epsilon_R - J^2/4 = 0 \) with the solution

\[ \hbar\Omega\pm = -\frac{\epsilon_L + \epsilon_R}{2} \pm \frac{\sqrt{J^2 + \Delta^2}}{2} , \quad (A.3) \]

where \( \Delta = \epsilon_R - \epsilon_L \) is the difference of the on-site chemical potentials. The amplitude in the right site can thus be written as the superposition \( c_R(t) = A_+ \exp(i\Omega_L t) + A_- \exp(i\Omega_- t) \). Inserting the initial conditions \( c_L(t = 0) = 1 \) and \( c_R(t = 0) = 0 \) into (A.1) and (A.2), respectively, we obtain \( \hbar\dot{c}_R(t = 0) = -J/2 \). These initial conditions for \( c_R \) and \( c_L \) lead to \( A_- = -A_+ \) and \( A_+ = J/(2\sqrt{\Delta^2 + J^2}) \), respectively. Thus we arrive at

\[ c_R(t) = \frac{J}{\sqrt{J^2 + \Delta^2}} \exp\left( -\frac{\epsilon_L + \epsilon_R}{2\hbar} t \right) \sin\left( \frac{\sqrt{J^2 + \Delta^2}}{2\hbar} t \right) \quad (A.4) \]

which implies the result (8) for \( p(t) = |c_R(t)|^2 \).

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