Mean-field dynamics of a non-hermitian Bose-Hubbard dimer

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We investigate an N-particle Bose-Hubbard dimer with an additional effective decay term in one of the sites. A mean-field approximation for this non-hermitian many-particle system is derived, based on a coherent state approximation. The properties of the resulting nonlinear, non-hermitian two-level system are analyzed, in particular the bifurcation scenario showing characteristic modifications of the self trapping transition. The mean-field dynamics is found to be in reasonable agreement with the full many-particle evolution.

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In the theoretical investigation of Bose-Einstein condensates (BEC) the celebrated mean-field approximation leading to the description via a nonlinear Schrödinger resp. Gross-Pitaevskii equation (GPE) is almost indispensable. It is usually achieved by replacing the bosonic field operators in the multi-particle system by c-numbers, the effective single-particle condensate wave functions, and describes the system quite well for large particle numbers and low temperatures. This approach is closely related to a classicalization [1, 2] and allows for the application of semiclassical methods [3–6].

Recently considerable attention has been paid to the description of scattering and transport behavior of BECs [7–10], as well as the implications of decay resp. boundary dissipation [11–13], phenomenologically described by effective non-hermitian mean-field theories. For linear quantum systems, an effective non-hermitian Hamiltonian formalism proved extremely useful and instructive for the description of open quantum systems in various fields of physics. Non-hermitian Hamiltonians typically yield complex eigenvalues whose imaginary parts describe the rates with which an eigenstate decays to the external world. Furthermore special kinds of non-hermitian quantum theories (sometimes called PT-symmetric) have actually been suggested as a generalization of quantum mechanics on the fundamental level (see, e.g., [14]).

However, the non-hermitian GPE has been formulated in an ad hoc manner as a generalization of the mean-field Hamiltonian and a derivation starting from a non-hermitian many particle system is required. Due to the relation to quantum classical correspondence, this is as well interesting in a more general context concerning the classical limit of effective non-hermitian quantum theories.

In the present paper we therefore provide a generalized mean-field approximation and investigate the characteristic features of the dynamics resulting from the interplay of nonlinearity and non-hermiticity for a simple many-particle Hamiltonian of Bose-Hubbard type, describing a BEC in a leaking double well trap:

$$\begin{aligned}\hat{\mathcal{H}} \;&=\; (\varepsilon - 2i\gamma)\hat{a}_1^\dagger \hat{a}_1 - \varepsilon \hat{a}_2^\dagger \hat{a}_2 + v(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_1 \hat{a}_2^\dagger)\\ &\quad + \frac{c}{2}(\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2)^2, \qquad (1)\end{aligned}$$

where $\hat{a}_j$, $\hat{a}_j^\dagger$ are bosonic particle annihilation and creation operators for the jth mode. The onsite energies are $\pm\varepsilon$, v is the coupling constant and c is the strength of the onsite interaction. The additional imaginary part of the mode energy γ models a decay, i.e., considers the first mode as a resonance state with a finite lifetime, like, e.g., the Wannier-Stark states for a tilted optical lattice [15]. A direct experimental realization could be achieved by tunneling escape of atoms from one of the wells. Even in the non-hermitian case, the Hamiltonian commutes with the total number operator $\hat{N} = \hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2$ and the number N of particles is conserved. The "decay" describes not a loss of particles but models the decay of the probability to find the particles in the two sites considered here.

First theoretical results for the spectrum of the non-hermitian two-site Bose-Hubbard system (1) and a closely related PT-symmetric system were presented in [16, 17]. In this paper we will present first results for the *dynamics* of this decaying many-particle system with emphasis on the mean-field limit of large particle numbers. In order to specify the mean-field approximation in a controllable manner, we derive coupled equations for expectation values under the assumption that the system, initially in a coherent state, remains in such a coherent state for all times of interest. This is a direct extension of the celebrated frozen Gaussian approximation in flat phase space (see, e.g., [18, 19]) to $SU(2)$ coherent states, relevant for the present case as discussed below. This yields classical evolution equations for the coherent states parameters.

It facilitates the analysis to rewrite the Hamiltonian (1) in terms of angular momentum operators (generators of the $SU(2)$-algebra)

$$\begin{aligned}\hat{L}_x = \tfrac{1}{2}(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_1 \hat{a}_2^\dagger), \qquad \hat{L}_y = \tfrac{1}{2i}(\hat{a}_1^\dagger \hat{a}_2 - \hat{a}_1 \hat{a}_2^\dagger),\\ \hat{L}_z = \tfrac{1}{2}(\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2), \qquad (2)\end{aligned}$$

satisfying the commutation rules $[\hat{L}_x, \hat{L}_z] = i\hat{L}_z$ and cyclic permutations, as

$$\hat{\mathcal{H}} = 2(\varepsilon - i\gamma)\hat{L}_z + 2v\hat{L}_x + 2c\hat{L}_z^2 - i\gamma\hat{N}. \qquad (3)$$

The conservation of $\hat{N}$ appears as the conservation of $\hat{L}^2 = \frac{\hat{N}}{2}\big(\frac{\hat{N}}{2}+1\big)$, i.e., the rotational quantum number $\ell = N/2$.

The system dynamics is therefore restricted to an $(N+1)$-dimensional subspace and can be described in terms of the Fock states $|k,N-k\rangle$, $k=0,\ldots,N$ or the $SU(2)$ coherent states [20], describing a pure BEC,

$$\begin{aligned} |x_1,x_2\rangle &= \frac{1}{\sqrt{N!}}\left(x_1\hat{a}_1^\dagger + x_2\hat{a}_2^\dagger\right)^N|0\rangle \\ &= \sum_{k=0}^{N}\binom{N}{k}^{1/2} x_1^k x_2^{N-k}|k,N-k\rangle, \end{aligned} \tag{4}$$

with $x_j\in\mathbb{C}$, whose normalization $\langle x_1,x_2|x_1,x_2\rangle = n^N$ with

$$n=|x_1|^2+|x_2|^2 \tag{5}$$

may differ from unity.

A general discussion of the time evolution of a quantum system under a non-hermitian Hamiltonian $\hat{\mathcal{H}}=\hat{H}-i\hat{\Gamma}$ with hermitian $\hat{H}$ and $\hat{\Gamma}$ can be found in [21]. Matrix elements of an operator $\hat{A}$ without explicit time-dependence satisfy the generalized Heisenberg equation, which in our case becomes

$$\begin{aligned} i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi|\hat{A}|\psi\rangle &= \langle\psi|\hat{A}\hat{\mathcal{H}}-\hat{\mathcal{H}}^\dagger\hat{A}|\psi\rangle \\ &= \langle\psi|\,[\hat{A},\hat{H}]\,|\psi\rangle - i\langle\psi|\,[\hat{A},\hat{\Gamma}]_+|\psi\rangle, \end{aligned} \tag{6}$$

where $[\ ,\ ]_+$ is the anti-commutator. As an immediate consequence of the non-hermiticity, the norm of the quantum state is not conserved:

$$\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi|\psi\rangle = -2\langle\psi|\hat{\Gamma}|\psi\rangle\,, \tag{7}$$

i.e. the survival probability decays exponentially for the simple case of a constant $\Gamma>0$. The time evolution of the expectation value of an observable $\langle\hat{A}\rangle=\langle\psi|\hat{A}|\psi\rangle/\langle\psi|\psi\rangle$ is described by the equation of motion

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{A}\rangle = \langle[\hat{A},\hat{H}]\rangle - 2i\,\Delta^2_{A\Gamma}\,, \tag{8}$$

with the covariance $\Delta^2_{A\Gamma}=\langle\frac{1}{2}[\hat{A},\hat{\Gamma}]_+\rangle-\langle\hat{A}\rangle\langle\hat{\Gamma}\rangle$.

For the Bose-Hubbard system (3) these evolution equations, formulated in terms of the angular momentum operators with $\hat{H}=2\varepsilon\hat{L}_z+2v\hat{L}_x+2c\hat{L}_z^2$ and $\hat{\Gamma}=\gamma(2\hat{L}_z+\hat{N})$, read (units with $\hbar=1$ are used in the following)

$$\begin{aligned} \tfrac{\mathrm{d}}{\mathrm{d}t}\langle\hat{L}_x\rangle &= -2\varepsilon\langle\hat{L}_y\rangle - 2c\langle[\hat{L}_y,\hat{L}_z]_+\rangle - 2\gamma\{2\Delta^2_{L_xL_z}+\Delta^2_{L_x,N}\} \\ \tfrac{\mathrm{d}}{\mathrm{d}t}\langle\hat{L}_y\rangle &= 2\varepsilon\langle\hat{L}_x\rangle + 2c\langle[\hat{L}_x,\hat{L}_z]_+\rangle - 2v\langle\hat{L}_z\rangle - 2\gamma\{2\Delta^2_{L_yL_z}+\Delta^2_{L_y,N}\} \\ \tfrac{\mathrm{d}}{\mathrm{d}t}\langle\hat{L}_z\rangle &= 2v\langle\hat{L}_y\rangle - 2\gamma\{2\Delta^2_{L_zL_z}+\Delta^2_{L_zN}\} \end{aligned} \tag{9}$$

and the norm decays according to

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi|\psi\rangle = -2\gamma\big\{2\langle\hat{L}_z\rangle+\langle\hat{N}\rangle\big\}\langle\psi|\psi\rangle. \tag{10}$$

In order to establish a mean-field description, we start from a system initially in a coherent state $|x_1,x_2\rangle$, i.e. a most classical state, and assume that the state remains coherent for all times of interest. This assumption is, in fact, exact, if the Hamiltonian is a linear superposition of the generators of the dynamical symmetry group, i.e. for vanishing interaction $c=0$ (the proof in [20] can be directly extended to the non-hermitian case). For the interacting case $c\neq 0$ this is an approximation and the mean-field equations of motion are obtained by replacing the expectation values in the generalized Heisenberg equations of motion (9) by their values in $SU(2)$ coherent states (4).

The $SU(2)$ expectation values of the $\hat{L}_i$, $i=x,y,z$ read

$$s_x=\frac{x_1^*x_2+x_1x_2^*}{2n}\ ,\ s_y=\frac{x_1^*x_2-x_1x_2^*}{2in}\ ,\ s_z=\frac{x_1^*x_1-x_2^*x_2}{2n}, \tag{11}$$

with the abbreviations $s_j=\langle\hat{L}_j\rangle/N$ for the mean values per particle and the expectation values of the anti-commutators factorize as

$$\langle[\hat{L}_i,\hat{L}_j]_+\rangle = 2\left(1-\frac{1}{N}\right)\langle\hat{L}_i\rangle\langle\hat{L}_j\rangle+\delta_{ij}\frac{N}{2}\,, \tag{12}$$

and $\langle[\hat{L}_i,\hat{N}]_+\rangle=2N\langle\hat{L}_i\rangle$. Inserting these expressions into (9) and taking the macroscopic limit $N\to\infty$ with $Nc=g$ fixed, we obtain the desired non-hermitian mean-field evolution equations:

$$\begin{aligned} \dot{s}_x &= -2\varepsilon s_y \ -4gs_zs_y \qquad\qquad +4\gamma s_zs_x, \\ \dot{s}_y &= +2\varepsilon s_x \ +4gs_zs_x \ -2vs_z \ +4\gamma s_zs_y, \\ \dot{s}_z &= \qquad\qquad\qquad\quad +2vs_y \ -\gamma(1-4s_z^2)\,. \end{aligned} \tag{13}$$

These nonlinear Bloch equations are real valued and conserve $s^2=s_x^2+s_y^2+s_z^2=1/4$, i.e. the dynamics is regular and the total probability n decays as

$$\dot{n}=-2\gamma(2s_z+1)\,n\,. \tag{14}$$

This mean-field approximation becomes exact for $g=0$ (provided that the initial state is coherent) and reduce to the well-known mean-field equations in the hermitian case $\gamma=0$.

Equivalently, the nonlinear Bloch equations (13) can be written in terms of a non-hermitian generalization of the discrete nonlinear Schrödinger equation, i.e., for the time-evolution of the coherent state parameters x_1, x_2. Most interestingly, these equations are canonical, $i\dot{x}_j=\partial H/\partial x_j^*$, $i\dot{x}_j^*=-\partial H^*/\partial x_j$, $j=1,2$, where the Hamiltonian function is related to the expectation value of the Hamiltonian $\hat{\mathcal{H}}$: $H(x_1,x_1^*,x_2,x_2^*)=\langle\hat{\mathcal{H}}\rangle n/N$ and can be conveniently rewritten in terms of the quantities $\psi_j=\mathrm{e}^{i\beta}x_j$ where the (insignificant) total phase is adjusted according to $\dot{\beta}=-g\kappa^2$ with $\kappa=(|\psi_1|^2-|\psi_2|^2)/n$. The resulting discrete non-hermitian GPE reads

$$i\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = \begin{pmatrix}\varepsilon+g\kappa-2i\gamma & v\\ v & -\varepsilon-g\kappa\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} \tag{15}$$

and the survival probability decays as $\dot{n}=-2\gamma(1-\kappa)n$. It should be pointed out that very similar non-hermitian mean-field equations, leading to different dynamics, have been suggested and studied before [11, 12, 16, 22] differing in the κ-term, which is there equal to $\kappa=|\psi_1|^2-|\psi_2|^2$. Note that these ad hoc nonlinear non-hermitian equations appear as well for absorbing nonlinear waveguides, see e.g. [23].

The dynamics of the nonlinear Bloch equations (13) is organized by the fixed points which are given by the real roots of the fourth order polynomial

$$4(g^2+\gamma^2)s_z^4+4g\varepsilon s_z^3+(\varepsilon^2+v^2-g^2-\gamma^2)s_z^2-g\varepsilon s_z-\varepsilon^2/4=0\,. \tag{16}$$

In the following we will restrict ourselves to the symmetric case $\varepsilon=0$. Then the polynomial (16) becomes biquadratic and the fixed points are easily found analytically.

In parameter space we have to distinguish three different regions: (a) For $g^2+\gamma^2<v^2$, we have two fixed points, which are both simple centers. (b) For $|\gamma|>|v|$, we have again two fixed points, a sink and a source. (c) Four coexisting fixed points are found in the remaining region, namely a sink and a source (resp. two centers for $\gamma=0$), a center and a saddle point. Note that the index sum of these singular points on the Bloch sphere must be conserved under bifurcations and equal to two [24]. Bifurcations occur at critical parameter values: For $g^2+\gamma^2=v^2$ (and $\gamma\neq 0$), one of the two centers (index $+1$) bifurcates into a saddle (index -1) and two foci (index $+1$), one stable (a sink) and one unstable (a source). This is a non-hermitian generalization of the selftrapping transition for $\gamma=0$. Note that the corresponding critical interaction strength is decreased by the non-hermiticity, i.e. the decay supports selftrapping . For $\gamma=\pm v$, the saddle (index -1) and the center (index $+1$) meet and disappear. For $g=0$, we observe a non-generic bifurcation at $\gamma=\pm v$ (an exceptional point [17]) where the two centers meet and simultaneously change into a sink and a source.

As an example, Fig. 1 shows the flow (11) on the Bloch sphere for $v=1$ both for the hermitian $\gamma=0$ (top) and the non-hermitian case $\gamma=0.75$ (bottom). For $\gamma=0$ we observe the well-known selftrapping effect: In the interaction free case $g=0$ (upper left) we have two centers at $s_y=s_z=0$,

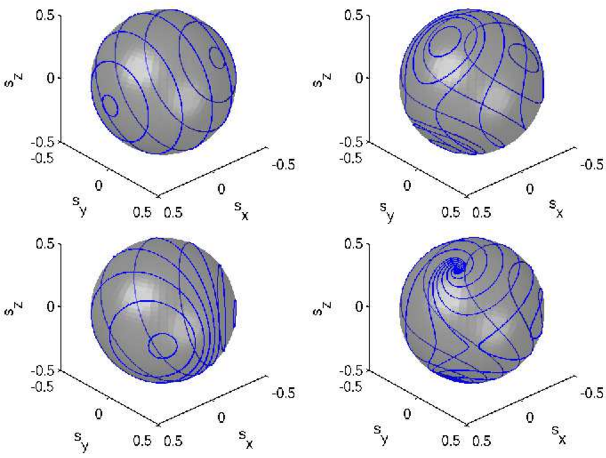

FIG. 1: (Color online) Mean-field dynamics on the Bloch sphere for the hermitian $\gamma=0$ (top) and the non-hermitian case $\gamma=0.75$ (bottom) for $g=0$ (left) and $g=2$ (right) and $\varepsilon=0$ and $v=1$.

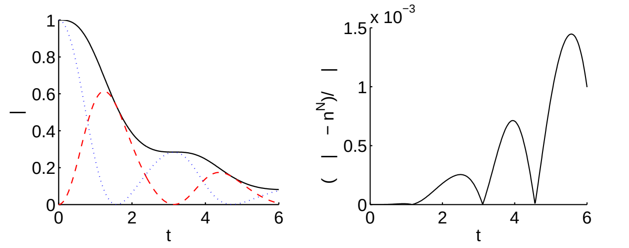

FIG. 2: (Color online) Decay of the survival probability (full black curve) and the populations of site 1 (dashed red curve) and 2 (dotted blue curve) for an initial coherent state located at the south pole, for $g=0.1$, $\gamma=0.01$, $v=1$ and $N=20$ (left) and the relative deviations between many-particle and mean-field results (right).

$s_x=\pm\frac{1}{2}$ and Rabi oscillations. Increasing the interaction g one of the centers bifurcates into a saddle (still at $s_z=0$) and two centers, which approach the poles with increasing g (upper right for $g=2$). The corresponding nonlinear stationary states therefore favor one of the wells. In the decaying system with $\gamma=0.75$ (bottom), these patterns are changed. For $g=0$ (lower left) we are still in region (a) with two centers located on the equator, however they move towards $s_x=0$, $s_y=\frac{1}{2}$, approaching each other. For $g=2$ (lower right), in region (b) above the bifurcation, we have a center, a sink (lower hemisphere), a source (upper hemisphere) and a saddle. The system relaxes to a state with excess population in the non-decaying well, i.e. the selftrapping oscillations are damped, which is in agreement with the effect of decoherence in a related nonlinear two mode system reported in [25]. Finally, in region (c) only a source and a sink survive and the flow pattern simplifies again (not shown). The manifestation of the different mean-field regimes in the many particle system is the occurrence and unfolding of higher order exceptional points in the spectrum [17].

Let us finally compare the mean-field evolution with the full many-particle dynamics. The full quantum solution is obtained by numerically integrating the Schrödinger equation for the Bose-Hubbard Hamiltonian (1) for an initial coherent state with unit norm.

Figure 2 shows the decay of the total survival probability $\langle\psi|\psi\rangle$ as a function of time for weak interaction, $g=0.1$, and weak decay, $\gamma=0.01$ with $v=1$, when initially the non-decaying site 2 is populated. The multi-particle results agree with the mean-field counterpart n^N on the scale of drawing. The deviation increases with time as can be seen on the right hand side. The probability shows a characteristic staircase behavior (see also [12, 13]) due to the fact that the population oscillates between the two sites and the decay is fast when site 1 is strongly populated and slow if it is empty. This picture is confirmed by the populations $\langle\psi|\hat a_1^\dagger\hat a_1|\psi\rangle/N$ and $\langle\psi|\hat a_2^\dagger\hat a_2|\psi\rangle/N$ of the two sites also shown in the figure. These quantities also agree with their mean-field counterparts $(1/2+s_z)n^N/2$ resp. $(1/2-s_z)n^N/2$ on the scale of drawing. The overall decay of the norm is approximately exponential, $\frac{d}{dt}\langle\psi|\psi\rangle\approx-2\gamma N\langle\psi|\psi\rangle$ within region (a), as seen from (14)

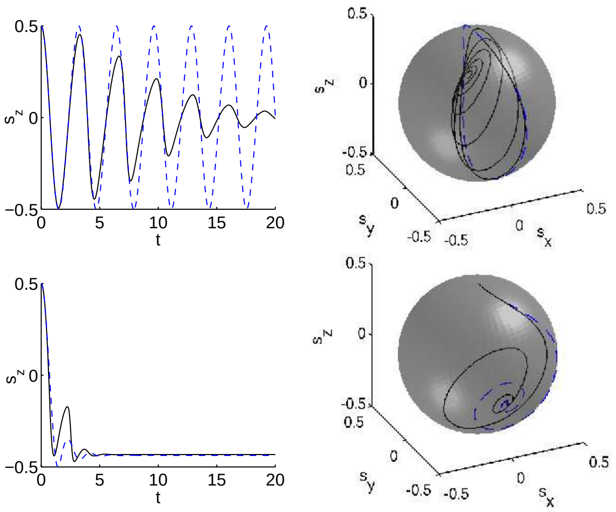

FIG. 3: (Color online) Mean-field evolution of the population imbalance $s_z(t)$ (dashed blue curve) in comparison with the full many particle system for $N = 20$ particles (black curve) for an initial coherent state located at the north pole. Parameters are $g = 0.5$ and $\gamma = 0.1$ (top) and $g = 2$ and $\gamma = 0.5$ (bottom) and $v = 1$.

with $\overline{s_z} = 0$.

The dynamics on the Bloch sphere in region (a) typically shows Rabi-type oscillations. An example for parameters $g = 0.5$ and $\gamma = 0.1$ is shown in Fig. 3. The classical mean-field oscillation follows a big loop extending over the whole Bloch sphere. The many-particle motion oscillates with the same period, however with a decreasing amplitude. This effect, known as breakdown of the mean-field approximation in the hermitian case, is due to the spreading of the quantum phase space density over the Bloch sphere and can be partially cured by averaging over a density distribution of mean-field trajectories as demonstrated in [26].

For strong interaction, i.e. in the selftrapping region (c), we find an attractive fixed point, a sink, in the mean-field dynamics. An example is shown in Fig. 3 for $g = 2$ and $\gamma = 0.5$. The mean-field trajectory, started at the north pole, approaches the fixed point at $s_{z,0} = -0.433$. The full many-particle system shows a very similar behavior.

Further numerical investigations show, that the short time behavior of the many-particle dynamics, as well as characteristic quantities as, e.g., the half-life time, are extremely well captured by the mean-field description in most parameter ranges. A more detailed discussion of the correspondence of the many-particle and the mean-field dynamics, especially concerning the limit of large particle numbers, is an interesting topic for future studies.

In this letter, we have constructed a mean-field approximation for a non-hermitian two-site multi-particle Bose-Hubbard Hamiltonian modeling a decaying system, which can directly be generalized to other effective non-Hermitian Hamiltonians. The resulting dynamics differ from the ad-hoc non-hermitian evolution equations used in previous studies. A comparison with exact results showed satisfying agreement. It should be noted, that a second approach is possible, based on a number-conserving evolution equation in quantum phase space formulated recently for M-site Bose-Hubbard systems [26], which allows for an immediate extension to the non-hermitian case.

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