Model of a \mathcal{PT} -symmetric Bose-Einstein condensate in a δ -function double-well potential

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The observation of \mathcal{PT} symmetry in a coupled optical waveguide system that involves a complex refractive index has been demonstrated impressively in the experiment by Rüter *et al.* [Nat. Phys. **6**, 192 (2010)]. This is, however, only an optical *analog* of a quantum system, and it would be highly desirable to observe the manifestation of \mathcal{PT} symmetry and the resulting properties also in a real, experimentally accessible, *quantum* system. Following a suggestion by Klaiman *et al.* [Phys. Rev. Lett. **101**, 080402 (2008)], we investigate a \mathcal{PT} -symmetric arrangement of a Bose-Einstein condensate in a double-well potential, where in one well cold atoms are injected while in the other particles are extracted from the condensate. We investigate, in particular, the effects of the nonlinearity in the Gross-Pitaevskii equation on the \mathcal{PT} properties of the condensate. To study these effects we analyze a simple one-dimensional model system in which the condensate is placed into two \mathcal{PT} -symmetric δ -function traps. The analysis will serve as a useful guide for studies of the behavior of Bose-Einstein condensates in realistic \mathcal{PT} -symmetric double wells.

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Beginning with the seminal paper by Bender and Boettcher in 1999 [1], parity-time (\mathcal{PT}) symmetric quantum mechanics has attracted ever-increasing attention over the past decade because it offers a class of complex Hamiltonians which, in spite of their non-Hermiticity, possess discrete real energy eigenvalue spectra. Moreover, these Hamiltonians feature the property of branch points, i.e., the coalescence of both energy values and eigenfunctions when some parameter in the Hamiltonian is varied, a phenomenon impossible in Hermitian quantum mechanics (but known to appear for resonances in the continuous spectrum; see, e.g., [2]).

Recently \mathcal{PT} symmetry has been realized experimentally in structured optical waveguides [3,4], where the complex index of refraction is manipulated by introducing loss and gain terms. These experiments make use of the quantum-optical analogy that the wave equation for the transverse electric field mode is formally equivalent to the one-dimensional Schrödinger equation. It would, however, be desirable to observe \mathcal{PT} symmetry also in a real quantum system.

Klaiman et al. [5] have suggested a quantum scenario analogous to the waveguide experiments in which a Bose-Einstein condensate is placed in a double-well potential, and loss and gain is realized by removing atoms in one well and coherently adding particles in the other. These authors pointed out that to have a close analogy with the optics experiments the nonlinearity in the Gross-Pitaevskii equation governing these condensates should be kept small. Here we want to ask the opposite question: What are the effects of the nonlinearity on the \mathcal{PT} symmetry on such an arrangement of a Bose-Einstein condensate? It is namely exactly the nonlinearity, proportional to $|\psi(x)|^2$, in the Gross-Pitaevskii equation that complicates matters. A necessary condition for the Hamiltonian to be \mathcal{PT} symmetric is that the imaginary part of the potential is an odd function and the real part an even function of x. The latter cannot be assumed from the outset for $|\psi(x)|^2$ when solving the Gross-Pitaevskii equation.

In this paper we will investigate the effects of the nonlinearity on the \mathcal{PT} symmetry in the spirit of a model calculation by considering the situation where the double well is idealized by two δ -function traps, with loss added in one trap and gain in the other. We will demonstrate that the stationary solutions of the Gross-Pitaevskii equation indeed preserve the \mathcal{PT} symmetry of the nonlinear Hamiltonian, and merge in a branch point at some critical value of the loss and gain, beyond which the symmetry is broken. Our results show that it will be a worthwhile enterprise to investigate \mathcal{PT} -symmetric Bose-Einstein condensates in realistic double-well potentials, and possibly pin down physical parameters where \mathcal{PT} breaking could be observed in a real experiment.

A model which mimics the physical situation of a BEC in a symmetric double well with loss and gain has already been investigated by Graefe *et al.* [6–8] in the framework of a twomode Bose-Hubbard-type \mathcal{PT} -symmetric Hamiltonian. As an optical analog, in the two-mode approximation Ramezani *et al.* [9] have recently looked at a mathematical model of a \mathcal{PT} symmetric coupled dual waveguide arrangement with Kerr nonlinearity. It is one objective of this paper to see which features of these models are recovered when actually solving the nonlinear \mathcal{PT} -symmetric Gross-Pitaevskii equation.

For a system where a real δ -function potential is augmented by a \mathcal{PT} -symmetric pair of δ functions with imaginary coefficients, bound states and scattering wave functions have been calculated by Jones [10]. His interest was devoted to the quasi-Hermitian analysis of the problem, and no nonlinearity was present. Jakubský and Znojil [11] have considered the explicitly solvable model of a particle exposed to two imaginary $\mathcal{PT}\delta$ -function potentials in an infinitely high square well, and determined the energy spectrum. The nonlinear Schrödinger equation for a δ -functions comb was studied by Witthaut *et al.* [12] with the aim of gaining insight into the properties of nonlinear stationary states of periodic potentials. Also, there exists a vast amount of literature on solitons and Bose-Einstein condensates in periodic optical and nonlinear lattices with \mathcal{PT} symmetry and their nonlinear optical analogs (see, e.g., [13-21]). But to the best of our knowledge the basic problem of two \mathcal{PT} -symmetric δ -function double wells with Gross-Pitaevskii nonlinearity has not been considered so far.

The Gross-Pitaevskii equation we analyze in this paper has the form

$$-\Psi''(x) - [(1+i\gamma)\delta(x+b) + (1-i\gamma)\delta(x-b)]\Psi(x)$$

$$-g|\Psi(x)|^2\Psi(x) = -\kappa^2\Psi(x), \qquad (1)$$

with $\kappa \in \mathbb{C}$, $\operatorname{Re}(\kappa) > 0$, and γ real. It consists of two δ -function traps with distance *a*, located at $b = \pm a/2$, with a real attractive part of the potential and imaginary gain-loss terms whose strengths are determined by the parameter γ , and a nonlinear term with amplitude *g*, which arises from the contact interaction of the condensate atoms. Units have been chosen in such a way that the strength of the real part of the δ -function potential is normalized to unity. While the δ -function potentials are \mathcal{PT} symmetric, it is not clear *a priori* that the equation itself is \mathcal{PT} symmetric since this requires the nonlinear term to be a symmetric function.

For vanishing nonlinearity, we find that the simple quantum mechanics model captures, for both eigenvalues and wave functions, all the effects of a \mathcal{PT} -symmetric waveguide configuration in optics. This is essentially due to the fact that two attractive δ -function potentials have exactly two bound states which correspond to the two supermodes in the waveguide arrangement.

For nonvanishing nonlinearity we have solved the Gross-Pitaevskii equation (1) numerically using a procedure in which the energy eigenvalues are found by a five-dimensional numerical root search. The free parameters which have to be adjusted in such a way that a physically meaningful wave function is obtained are the eigenvalue κ as well as initial conditions for the wave function and its derivative. Since the overall phase is arbitrary we can choose it such that $\Psi(0)$ is a real number. Therefore five real parameters remain, viz., the real part of $\Psi(0)$ and the real and imaginary parts of both $\Psi'(0)$ and κ . Physically relevant wave functions must be square integrable and normalized. The normalization is important since the Gross-Pitaevskii equation is nonlinear and the norm influences the Hamiltonian. This gives in total five conditions which have to be fulfilled: The real and imaginary parts of Ψ must vanish for $x \to \pm \infty$, and the norm of the wave function must fulfill $||\psi|| - 1 = 0$.

Outside the δ -function traps the Gross-Pitaevskii equation (1) coincides with the free nonlinear Schrödinger equation, which has well-known real solutions in terms of Jacobi elliptic functions (cf., e.g., [12,22,23]). The function which solves the equation in the ranges |x| > b for the attractive nonlinearity considered here and decays to zero for $|x| \rightarrow \infty$ is $cn(\kappa x, 1) = 1/cosh(\kappa x)$. We find that once the correct eigenvalues and eigenfunctions are obtained our numerical wave functions exactly show this behavior.

Figure 1 shows the results for the eigenvalues κ calculated for a value of the nonlinearity parameter g = 1.0 and a trap distance of a = 2.2 as functions of γ . The results for the case g = 0 are also shown for comparison. It can be seen that even with nonlinearity there still exist two branches of real eigenvalues up to a critical value $\gamma_{cr} \approx 0.4$, at which the two eigenvalues coincide. There also appears a branch of two complex conjugate eigenvalues, but surprisingly these are born, not at γ_{cr} , but at the smaller value of $\gamma \approx 0.31$ where they bifurcate from the real eigenvalue branch of the ground

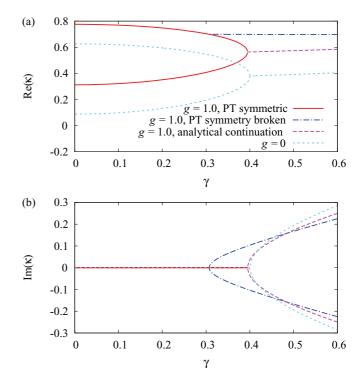


FIG. 1. (Color online) Eigenvalues κ of the nonlinear equation (1) as functions of the size of the loss-gain parameter γ for a = 2.2. The value of the nonlinearity parameter chosen is g = 1. The case g = 0 is drawn (dashed lines) for comparison. A branch of complex conjugate eigenvalues appears which bifurcates from the ground-state branch before the critical value of γ where the branches of the real eigenvalues coalesce in an exceptional point. There a pair of complex eigenvalues only emerges after an analytical continuation of the nonlinearity in the Gross-Pitaevskii equation. All quantities are plotted dimensionless.

state. This implies that there is a range of γ values where two real and two complex eigenvalues coexist.

At this point it is useful to establish a link with the model of a \mathcal{PT} -symmetric Bose-Hubbard dimer with loss and gain investigated by Graefe et al. [8]. An eigenenergy spectrum with a structure similar to the one in Fig. 1 also appeared in their calculations (see Fig. 13 in Ref. [8]). In the model, stationary states correspond to fixed points of the motion of a vector on the surface of the Bloch sphere, whose types can be classified according to the eigenvalues of the Jacobian matrix. In the region where only two real eigenvalues exist the solutions correspond to centers, while in the region with four eigenvalues the solutions correspond to a center and a saddle point, and a sink and a source. The center and saddle point collide at the branch point and vanish. This behavior is in complete agreement with the results shown in Fig. 1. It may be concluded that the familiar branching scheme known for \mathcal{PT} -symmetric Hamiltonians quite generally will be changed into a scheme of the type as shown in Fig. 1 if a nonlinearity is added to the Hamiltonian.

Figure 2 shows the real and imaginary parts of the ground state and the excited state determined numerically for g = 1, a = 2.2, and $\gamma = 0.35$, below the the critical value $\gamma_{cr} \approx 0.4$. The \mathcal{PT} symmetry of each wave function is evident since their real parts are even functions and their imaginary parts odd

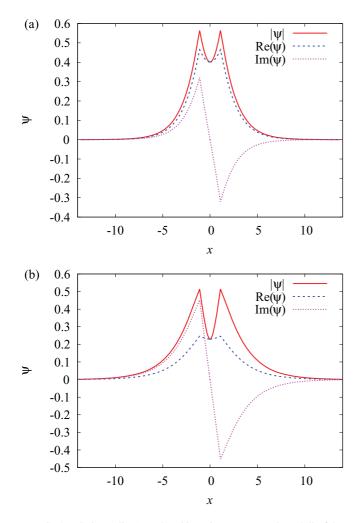


FIG. 2. (Color online) Real and imaginary parts and moduli of the eigenstates of the nonlinear Hamiltonian in Eq. (1) for g = 1, a = 2.2, and $\gamma = 0.35$, (a) ground state and (b) excited state. The wave functions are \mathcal{PT} symmetric, and the moduli are symmetric functions, producing the \mathcal{PT} symmetry of the total nonlinear Hamiltonian. All quantities are plotted dimensionless.

functions of x. From the \mathcal{PT} symmetry of the wave function follows that the modulus, also shown in Fig. 2, is an even function, and with it the nonlinear term in Eq. (1). We therefore have the important result that the nonlinear Hamiltonian picks as eigenfunctions exactly those states in Hilbert space which render the nonlinear Hamiltonian \mathcal{PT} symmetric. In the ground state, which emerges from the symmetric real wave function for $\gamma = g = 0$, the symmetric contribution from the real part still dominates, while for the excited state, which originates from the antisymmetric solution for $\gamma = g = 0$, the antisymmetric contribution from the imaginary part prevails.

The \mathcal{PT} symmetry of the wave functions is broken for the eigenstates with complex eigenvalues. Figure 3 shows as an example the wave functions obtained for g = 1, a = 2.2, and $\gamma = 0.5$ for the corresponding pair of complex conjugate eigenvalues κ . It can be seen that the real and imaginary parts are no longer even or odd functions, and therefore \mathcal{PT} symmetry is lost. As a consequence, the moduli of the wave functions also are no longer even functions of x. Thus we find that

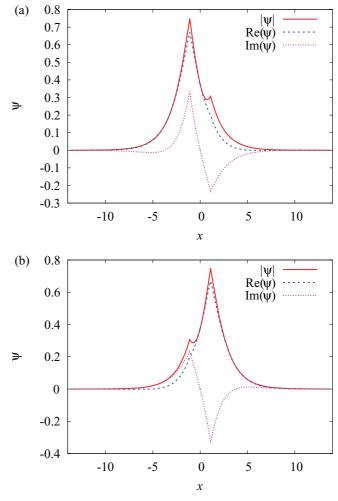


FIG. 3. (Color online) Real and imaginary parts and moduli of the eigenstates of the nonlinear Hamiltonian in Eq. (1) for g = 1, a = 2.2, and $\gamma = 0.5$, (a) solution with imaginary part of $\kappa > 0$ and (b) imaginary part of $\kappa < 0$. The \mathcal{PT} symmetry is broken, the moduli are not symmetric functions, and the \mathcal{PT} symmetry also of the nonlinear Hamiltonian is broken. All quantities are plotted dimensionless.

beyond the branch point not only the \mathcal{PT} symmetry of the wave functions is broken but also that of the nonlinear Hamiltonian.

For the states with complex eigenvalues there is, however, an important difference between the case with and without nonlinearity: For complex eigenvalues the modulus squared of the wave functions grows or decays proportional to $\exp[-2\text{Im}(\kappa^2)t]$, and so does the nonlinear term in Eq. (1). Therefore the solutions presented here are not true stationary states of the time-dependent Gross-Pitaevskii equation. However, $Im(\kappa^2)$ correctly describes the *onset* of the temporal evolution of the two modes as can be verified by inserting the eigensolutions with complex eigenvalues as initial wave functions into the time-dependent Gross-Pitaevskii equation and letting them evolve in time. Even though in the \mathcal{PT} -broken regime all initial wave functions will finally explode since the increase of particles in the well with gain will always dominate for long times, the influence of the two solutions with complex eigenvalues is always observable for $\text{Im}(\kappa^2)t \ll 1$ and initial wave functions not deviating much from the two eigenstates.

In Fig. 3 the mode with positive imaginary part of κ is the one which begins to decay—as expected it is more strongly localized in the trap with loss—while the mode with negative imaginary part is the one which starts to grow and is more strongly localized in the trap with gain.

The fact that at the branch point two real solutions coalesce without giving rise to two solutions with complex eigenvalues contradicts the usual behavior seen at exceptional points. Obviously these solutions cannot be found by solving the nonlinear Gross-Pitaevskii equation in its form (1), but require an analytical continuation of the nonlinear Hamiltonian beyond the critical point γ_{cr} . The reason is that the nonlinear term $g|\Psi|^2$ is a nonanalytic function, and some care has to be taken when analytically continuing the Hamiltonian beyond the exceptional point.

In the \mathcal{PT} -symmetric regime up to γ_{cr} we have $\Psi^*(x) = \Psi(-x)$. Therefore on the way to the bifurcation point we can write the nonlinearity for the \mathcal{PT} -symmetric states in the form $g|\Psi(x)|^2 \equiv g\Psi(x)\Psi(-x)$. This function can be continued analytically. In the numerical calculation the additional condition $\int \Psi(x)\Psi(-x)dx = 1$ must be introduced to fix the phase of the nonlinearity in the \mathcal{PT} -broken regime. In the (then) six-dimensional root search also Im[$\Psi(0)$] must be varied. As a result we find two more complex conjugate solutions that emerge from the coalescing states; see Fig. 1. These states are not \mathcal{PT} symmetric and no longer possess vanishing imaginary parts at the origin.

In this paper we have analyzed the simple quantum mechanical model of a Bose-Einstein condensate in \mathcal{PT} -symmetric δ -function double traps by directly solving the nonlinear Gross-Pitaevskii equation. We find two stationary eigenstates with real eigenvalues which at a critical value of the loss-gain parameter merge in a branch point. We have the important result that the wave functions are \mathcal{PT} symmetric. As a consequence their moduli are even functions, and therefore the nonlinear Hamiltonian selects as solutions exactly such states which make itself \mathcal{PT} symmetric. We also find a branch of two complex conjugate eigenvalues for which the \mathcal{PT} symmetry of the wave functions is broken, and with it that of the nonlinear Hamiltonian.

An unexpected result is that, with the nonlinearity present, the branches of complex conjugate eigenvalues do not bifurcate from the point where the real eigenvalues coincide, but emerge at a smaller value of the gain-loss term from the eigenvalue branch of the ground state. On the other hand, at the critical value of the gain-loss parameter we find the behavior characteristic of a branch point, i.e., the coalescence of both eigenvalues and eigenfunctions, but no pair of complex conjugate eigenvalues seems to emerge. These are found only after continuing analytically the nonlinear term in the Gross-Pitaevskii equation. Note, however, that as stated before, for complex eigenvalues the squared modulus of the wave function becomes time dependent, and a description using the stationary Gross-Pitaevskii equation breaks down anyway. This does not, however, affect the main result of our paper, namely the existence of \mathcal{PT} -symmetric eigenfunctions and the \mathcal{PT} symmetry of the Hamiltonian also when the nonlinearity is present.

We have considered the case of an attractive nonlinearity but found that the same behavior occurs for repulsive nonlinearity.

The results of our model calculation make one expect that similar \mathcal{PT} behavior should also prevail in Bose-Einstein condensates in more realistic double wells [24] with \mathcal{PT} symmetry, in one or more dimensions. Also, in addition to the nonlinearity resulting from the short-range contact interaction, condensates with a long-range dipole-dipole interaction [25] could be considered. Investigations of the Gross-Pitaevskii equation in these directions are under way. It would also be interesting to extend the quasi-Hermitian analysis given by Jones [10] and to investigate whether for the nonlinear \mathcal{PT} -symmetric Hamiltonian considered in the present paper the construction of a metric operator is possible with respect to which the nonlinear Hamiltonian is quasi-Hermitian. Furthermore it would be worthwhile looking for simple matrix models which show the behavior of the eigenvalues found for finite nonlinearity.

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