Nonlinear Schrödinger equation for a $\mathcal{PT}$-symmetric delta-function double well

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Received 30 March 2012
Published 23 October 2012
Online at stacks.iop.org/JPhysA/45/444008

Abstract

The time-independent nonlinear Schrödinger equation is solved for two attractive delta-function-shaped potential wells where an imaginary loss term is added in one well, and a gain term of the same size but with opposite sign in the other. We show that for vanishing nonlinearity the model captures all the features known from studies of parity–time ($\mathcal{PT}$-) symmetric optical waveguides, e.g., the coalescence of modes at an exceptional point at a critical value of the loss/gain parameter, and the breaking of $\mathcal{PT}$ symmetry beyond. With the nonlinearity present, the equation is a model for a Bose–Einstein condensate with loss and gain in a double-well potential. We find that the nonlinear Hamiltonian picks as stationary eigenstates exactly such solutions which render the nonlinear Hamiltonian itself $\mathcal{PT}$ symmetric, but observe coalescence and bifurcation scenarios different from those known from linear $\mathcal{PT}$-symmetric Hamiltonians.

This article is part of a special issue of Journal of Physics A: Mathematical and Theoretical devoted to ‘Quantum physics with non-Hermitian operators’.

PACS numbers: 03.65.Ge, 03.75.Hh, 11.30.Er

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

1. Introduction

The observation of parity–time ($\mathcal{PT}$) symmetry in experiments with structured optical waveguides [1, 2] marked a remarkable triumph for the mathematical theory of non-Hermitian Hamiltonians having $\mathcal{PT}$ symmetry, initiated by Bender and Boettcher [3] in 1999. The experiments exploit the optical–quantum mechanical analogy that the wave equation for the transverse electric field mode is formally equivalent to the one-dimensional Schrödinger equation when the potential is identified with $V(x) = -k^2n^2(x)$ and the energy eigenvalue with $E = -\beta^2$, where $k = \omega/c$ is the vacuum wave number and $\beta$ is the propagation constant of the mode. A $\mathcal{PT}$-symmetric experiment is realized by introducing loss and gain terms in the complex index of refraction $n(x)$.
A quantum analogue to the optical experiments would be a Bose–Einstein condensate in a double-well potential where loss and gain are realized by removing atoms from one well and pumping in atoms in the other, as has been suggested by Klaiman et al [4]. A complication arises from the interaction between the condensate atoms. In the simplest case this is s-wave scattering, which yields an additional (real-valued) potential term proportional to $|\psi|^2$, and turns the non-Hermitian Hamiltonian into a nonlinear one. For the Hamiltonian to be $\mathcal{PT}$ symmetric this term has to be a symmetric function of the coordinates, which cannot be guaranteed from the outset. It will be the purpose of this paper to analyse whether or not the nonlinearity destroys the $\mathcal{PT}$ symmetry of the quantum system.

We will do this, in the spirit of a model calculation, by considering the situation where the double well is idealized by two attractive delta-function potential wells, 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 at a branch point at some critical value of the loss and gain, beyond which the $\mathcal{PT}$ symmetry is broken.

Another model which simulates the physical situation of a Bose–Einstein condensate in a double well with loss and gain has been investigated by Graefe et al [5–7] in the framework of a two-mode Bose–Hubbard-type $\mathcal{PT}$-symmetric Hamiltonian. In the model, the dynamics of the quantum system is mapped on that of a (formal) spin vector whose motion on the surface of the Bloch sphere can be analysed in terms of classical nonlinear dynamics. As an optical analogue, in the two-mode approximation Ramezani et al [8] have recently looked at a mathematical model of a $\mathcal{PT}$-symmetric-coupled dual waveguide arrangement with Kerr nonlinearity. It will be interesting to see which features of these models are recovered when actually solving the nonlinear $\mathcal{PT}$-symmetric Gross–Pitaevskii equation.

Delta-function potentials are popular as model systems in the literature since they allow for analytic or partially analytic solutions but are flexible enough to provide insight into characteristic phenomena of more complex physical situations. For example, resonances and the decay behaviour of a Bose–Einstein condensate in a double delta-shell potential were analysed by Rapedius and Korsch [9] with the aim of modelling features typical of double-well potentials [10]. In the same vein, Witthaut et al [11] have studied the nonlinear Schrödinger equation for a delta-function comb to gain an insight into the properties of nonlinear stationary states of periodic potentials. For a system where a real delta-function potential is augmented by a $\mathcal{PT}$-symmetric pair of delta-functions with imaginary coefficients, bound states and scattering wavefunctions have been calculated by Jones [12]. The paper was devoted to the quasi-Hermitian analysis of the problem, and no nonlinearity was present. Jakubský and Znojil [13] 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, but also without nonlinearity. A large body of literature of course exists on the properties of solitons and Bose–Einstein condensates in periodic optical and nonlinear lattices with $\mathcal{PT}$ symmetry and their nonlinear optical analogues (see, e.g., [14–22]). But to the best of our knowledge the basic problem of the nonlinear Schrödinger equation with two $\mathcal{PT}$-symmetric delta-function double wells has not been treated so far.

2. Delta-function trap model

We consider a Bose–Einstein condensate trapped in two delta-function-shaped potential wells located at $x = \pm a/2$, where from one well condensate atoms are removed and the same number of atoms is added to the other. At sufficiently low temperatures, stationary solutions
for the condensate wavefunction are then described in a mean-field approach by the nonlinear Schrödinger equation, or the Gross–Pitaevskii equation (see, e.g., [23]),

\[-\Psi''(x) - [(1 + iy)\delta(x + a/2) + (1 - iy)\delta(x - a/2)]\Psi(x) - g|\Psi(x)|^2\Psi(x) = -\kappa^2\Psi(x),\]

where \(g\) is the nonlinear interaction strength, and the real-valued parameter \(\gamma\) determines the size of the gain and loss terms. Units have been chosen in such a way that the strength of the gain and loss terms. Beyond the branch point the eigenvalues become complex, and the real part of the delta-function potentials is normalized to unity. (The relation to physical quantities is given in the appendix.) For stationary solutions the eigenvalues \(\kappa\) will be real, but since we are interested in the complete eigenvalue spectrum, including complex eigenvalues, we will quite generally search for solutions with \(\kappa \in \mathbb{C}\), \(\text{Re}(\kappa) > 0\). While the delta-function potentials are \(\mathcal{PT}\) symmetric, it is not clear \textit{a priori} that the equation itself is \(\mathcal{PT}\) symmetric since this requires the nonlinear potential term to be a symmetric function of \(x\).

To be in a position to study the effects that emerge when the nonlinearity is turned on we first consider the case where the nonlinearity is absent, and then proceed to values \(g > 0\).

2.1. Delta-function trap model for vanishing nonlinearity

For \(g = 0\), the bound-state wavefunction has the following form:

\[
\Psi(x) = \begin{cases} 
A e^{sx} & : \quad x < -b \\
C e^{sx} + D e^{-sx} & : \quad -b < x < b \\
B e^{-sx} & : \quad b < x,
\end{cases}
\]

with \(b = a/2\). Applying the continuity conditions leads to the system of linear equations (with the abbreviation \(\kappa_0 = 1 + iy\)),

\[
\begin{align}
\kappa_0 e^{-sx}C + (\kappa_0 - 2\kappa)e^{sx}D &= 0, \\
(\kappa_0^* - 2\kappa)e^{sx}C + \kappa_0 e^{-sx}D &= 0.
\end{align}
\]

The eigenvalues \(\kappa\) are obtained numerically by finding the roots of the complex secular equation

\[
(1 + \gamma^2) e^{-2\kappa x} - (1 + \gamma^2 + 4\kappa^2 - 4\kappa) = 0.
\]

It depends on two parameters, the distance \(a\) of the traps and the strength \(\gamma\) of the loss/gain terms.

In figure 1, the eigenvalues \(\kappa\) are plotted as functions of the strength of the loss/gain parameter \(\gamma\) for different distances of the traps. It can be seen that the solutions exhibit the behaviour typical of \(\mathcal{PT}\)-symmetric non-Hermitian Hamiltonians: up to a critical value of the loss/gain parameter \(\gamma\) there exist two real eigenvalues \(\kappa\). Since we have included a minus sign on the right-hand side of the eigenvalue equation (1), in the range of real eigenvalues, the upper branch belongs to the ground state and the lower branch to an excited state. At the critical value—the branch point (or exceptional point)—the eigenvalues and the eigenfunctions merge. Beyond the branch point the eigenvalues become complex, and complex conjugate. The time dependence of the eigenstates of (1) with \(g = 0\) is given by \(\exp(\kappa x) \exp(\kappa x)\) (with \(k_l\) and \(k_i\) being the real and imaginary parts of \(\kappa\)); hence, the mode with \(k_i > 0\) decays and the mode with \(k_i < 0\) grows.

Of course, at \(\gamma = 0\), the two states turn into the well-known \(\cosh(\kappa x)\) (ground state) and \(\sinh(\kappa x)\) (excited state) textbook solutions of (1) between the traps. It is also well known that for \(\gamma = 0\), the excited state disappears at a distance of \(a = 2\). From figure 1(b) we see, however, that for \(a = 2\) an excited state is born as soon as loss/gain parameter is switched on. The figure also shows that for distances below \(a = 2\) (cf figure 1(c)) the excited state is born when loss and gain exceed a finite threshold value.

\[
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\]
Figure 1. Eigenvalues $\kappa$ of equation (1) for vanishing nonlinearity as functions of the size of the loss/gain parameter $\gamma$ for different distances of the delta-function traps: (a) $a = 2.2$, (b) $a = 2.0$, (c) $a = 1.8$.

The behaviour of the eigenvalues shown in figure 1 is in complete analogy with that found by Klaiman et al in their study of two micro waveguides with loss and gain (cf figure 2 in [4]). Their calculation was performed for a fixed distance of the waveguides. It would be interesting to investigate whether or not the excited mode also vanishes when the distance of the waveguides is decreased.

Below the branch point the wavefunctions possess $\mathcal{PT}$ symmetry, $\Psi^*(x) = \Psi(-x)$. In our model, this can be easily seen since for real $\kappa$ the complex conjugate of (2) is identical to (3) so that the pairs $(C, D)$ and $(D^*, C^*)$ fulfil the same equation, and, hence, $D = C^*$. From the continuity condition it then follows that $A = C + C^* e^{2i\kappa b}$ and $B = C e^{2i\kappa b} + C^* = A^*$. Note that quite generally the $\mathcal{PT}$ symmetry of a wavefunction implies that its modulus is a symmetric function, since $\Psi^*(x)\Psi(x) = \Psi(-x)\Psi^*(-x)$. 

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Figure 2 shows, for $a = 2.2$, the ratio of the coefficients $C$ and $D$ of the wavefunctions in dependence on the loss/gain parameter $\gamma$. What is shown is the evolution of the modulus of the ratio and its phase for the ground state and the excited state. Since below the branch point we have $D = C^* = |C| \exp(-i\varphi)$, the modulus of the ratio is 1, and its phase is twice the phase $\varphi$ of the coefficient $C$. As it must, at $\gamma = 0$ the phase starts with a value of 0 for the (symmetric) ground state and $\pi$ for the (antisymmetric) excited state. While the phase for the ground state is quickly rotated away from its initial value, the phase of the ratio belonging to the excited state only slowly deviates from $\pi$ up to the branch point. At the branch point, the modulus and the phase of $D/C$ coincide. Beyond the branch point they quickly evolve away from the values they have in the $PT$-symmetric regime.

It is instructive to look at the time dependence of a superposition of the two eigenstates in the $PT$-symmetric regime. For different values of the loss/gain parameter figure 3 shows the time evolution of

$$|\Psi(x, t)|^2 = |\psi_1(x) \exp(i\kappa_1^2 t) + \psi_2(x) \exp(i\kappa_2^2 t)|^2.$$

Without the loss/gain term, the probability density oscillates between the two delta-function wells. For finite gain and loss the beat frequency decreases and the oscillation is deformed, and for a loss/gain parameter close to the branch point the probability density on both sides is almost identical and pulsates. This behaviour completely agrees with the time evolution of the power distribution for a propagating electric sum field consisting of two guided modes calculated by Klaiman et al (cf figure 3 in [4]).
Figure 3. Time evolution of a superposition of the two eigenstates for different values of the loss/time parameter: (a) $\gamma = 0$, (b) $\gamma = 0.35$ and (c) $\gamma = 0.39$ close to the exceptional point.

Thus we find that the simple quantum mechanical model studied in this section already captures, for both eigenvalues and wavefunctions, all the effects of a $\mathcal{PT}$-symmetric waveguide configuration in optics.

2.2. Delta-function trap model with nonlinearity

2.2.1. Numerical method. For $g \neq 0$ 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 wavefunction is obtained are the eigenvalue $\kappa$ as well as initial conditions for the wavefunction 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, namely the real part of $\Psi(0)$, and the real and imaginary parts of both $\Psi'(0)$ and $\kappa$. Physically relevant wavefunctions must be square integrable and normalized. The normalization is important since the Gross–Pitaevskii equation is nonlinear and the norm influences the form of the Hamiltonian. This gives in total five conditions which have to be fulfilled. The real and imaginary parts of $\Psi$ must vanish for $x \to \pm \infty$, and the norm of the wavefunction must fulfill $||\psi|| - 1 = 0$.

Outside the delta-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., [11, 24, 25]). The function which solves the equation in the ranges $|x| > a/2$ for the attractive nonlinearity considered here and decays to zero for $|x| \to \infty$ is $\text{cn}(\kappa x, 1) = \text{sech}(\kappa x) = 1/\cosh(\kappa x)$. We find that once the correct eigenvalues and eigenfunctions are obtained our numerical wavefunctions show exactly this behaviour.
2.2.2. Eigenvalues. Figure 4 shows the results for the real and imaginary parts of the eigenvalues $\kappa$ calculated for a trap distance of $a = 2.2$ and different values of the nonlinearity parameter as functions of $\gamma$. The results for the case $g = 0$ are shown for comparison. It can be recognized that even with the nonlinearity present there always exist two branches of real eigenvalues, up to critical values $\gamma_{cr}$, where the two branches merge. It can also be seen that branches of two complex conjugate eigenvalues also appear, but it comes as a surprise that these are born, not at $\gamma_{cr}$, but at smaller values of $\gamma$ where they bifurcate from the real eigenvalue branch of the ground state. As the nonlinearity is increased, the bifurcation points are shifted to smaller values of $\gamma$, while the branches of the real eigenvalues practically retain their form and are shifted upwards. We therefore find that for non-vanishing nonlinearity, there always exists a range of $\gamma$ values where two real and two complex eigenvalues coexist.

This behaviour obviously is a new effect, caused by the nonlinearity in the Gross–Pitaevskii equation. In fact the different branches can be continuously transformed into each other: when, for fixed $\gamma$, we increase the nonlinearity from $g = 0$ in small steps to $g = 1$ and always take the solution of the previous step as input for the root search in the next step, the branch of complex conjugate eigenvalues which exists for $g = 0$ is continuously transferred to the branch of complex eigenvalues for $g = 1$ as shown in figure 4. Likewise, starting from the branch of complex conjugate eigenvalues for $g = 1$ at any value of $\gamma$ in the range where four
solutions exist and decreasing $g$ in small steps to $g = 0$ we end up on the branch belonging to the real eigenvalue of the ground state.

At this point, it is useful to compare the results of the investigations of a $\mathcal{PT}$-symmetric two-mode Bose–Hubbard Hamiltonian with loss and gain by Graefe et al [7]. An eigenenergy spectrum with a structure similar to the one shown in figure 4 also appeared in their calculations (see figure 13 in [7]). In the model, stationary states correspond to fixed points of the motion of a vector on 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 fixed points can be identified as centres, while in the region with four eigenvalues the fixed points correspond to a centre, a saddle point, a sink and a source. The centre and saddle point collide at the branch point and vanish.

This behaviour is in good agreement with the results shown in figure 4. A stability analysis of the wavefunctions shows that up to the bifurcation point both the ground state and the excited state are stable, they correspond to the two centres. Beyond the bifurcation point, the excited state remains stable (a centre) while the ground state becomes unstable (a saddle point). Out of the wavefunctions belonging to the two complex conjugate eigenvalues one decays and the other grows, corresponding to the sink and the source, respectively. It is gratifying that the two so different approaches qualitatively yield the same behaviour.

It can be concluded that quite generally the familiar branching scheme for linear $\mathcal{PT}$-symmetric Hamiltonians will be changed into a scheme of the type shown in figure 4 if a nonlinearity is added to the Hamiltonian.

2.2.3. Eigenfunctions. In figure 5, we present examples of wavefunctions of the eigenstates of the nonlinear Schrödinger equation (1) determined numerically for $g = 0.5$ and $a = 2.2$. The results for the ground state and the excited state are shown in figure 5(a) and (b) for $\gamma = 0.35$, below the critical value $\gamma_{cr} \approx 0.4$. The fact that in the numerical calculation the global phase of the complex wavefunction was fixed in such a way that $\Psi(0)$ is real makes it particularly easy to recognize the $\mathcal{PT}$ symmetry of the two solutions, since their real parts become even functions and their imaginary parts odd functions of $x$. From the $\mathcal{PT}$ symmetry of the wavefunction it follows that the modulus, also shown in figure 5, is an even function, and with it the nonlinear term in (1). We therefore have the important result that the nonlinear Schrödinger equation with loss and gain selects 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 wavefunction 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 wavefunctions is broken for the eigenstates with complex eigenvalues. Figures 5(c) and (d) show as examples the wavefunctions obtained for $\gamma = 0.5$ for the corresponding pair of complex conjugate eigenvalues $\kappa$. 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 wavefunctions also are no longer even functions of $x$. Thus, we find that beyond the branch point not only the $\mathcal{PT}$ symmetry of the wavefunctions is broken but also that of the nonlinear Hamiltonian!

It must be noted, however, that eigenstates with complex eigenvalues, in spite of solving the nonlinear eigenvalue problem (1), do not obey the corresponding time-dependent nonlinear Schrödinger equation. For complex eigenvalues the modulus squared of the wavefunctions grows or decays proportional to $\exp(-2\text{Im}(\kappa^2)t)$, and so does the nonlinear term in (1). Therefore strictly speaking multiplying these eigenstates with the usual time evolution factor
Figure 5. Real and imaginary parts and moduli of wavefunctions of the eigenstates of the nonlinear Hamiltonian in (1) for $g = 0.5, a = 2.2$. (a) Ground state and (b) excited state for $\gamma = 0.35$. (c) solution with imaginary part of $\kappa > 0$ and (d) imaginary part of $\kappa < 0$ for $\gamma = 0.5$. In (a) and (b), the wavefunctions are $\mathcal{PT}$ symmetric, and the moduli are symmetric functions, producing the $\mathcal{PT}$ symmetry of the total nonlinear Hamiltonian. The wavefunctions in (c) and (d) are no longer $\mathcal{PT}$ symmetric, their moduli are not symmetric functions, and the $\mathcal{PT}$ symmetry of the nonlinear Hamiltonian is also broken.

$\exp(i\kappa^2 t)$ only captures the onset of the temporal evolution of the two modes, for times $\text{Im}(\kappa^2 t) \ll 1$. If one wished to obtain the exact time evolution of these solutions in the region beyond the branch point, one would have to solve the time-dependent nonlinear Schrödinger equation (see subsection 2.2.5). In figure 5(c) the mode with positive imaginary part of $\kappa$ is the one which decays, as expected it is more strongly localized in the trap with loss, while the mode with negative imaginary part in figure 5(d) is the one which grows and is more strongly localized in the trap with gain.

To demonstrate that at $\gamma_{cr}$ the two eigenstates with real eigenvalues indeed coalesce, we have plotted their wavefunctions in figure 6 for $a = 2.2, g = 0.5$, close to the critical value of $\gamma_{cr} \approx 0.4$. While slightly below the critical value minor deviations of the wavefunctions are still visible, in particular in the imaginary parts, no differences can be recognized anymore at $\gamma = 0.398$. Thus also for strong nonlinearity at $\gamma_{cr}$ we find the properties characteristic of an exceptional point, i.e. the coalescence of both eigenvalues and eigenfunctions.

2.2.4. Analytical continuation of the nonlinear Hamiltonian. The fact that at the branch point two real solutions coalesce without giving rise to two solutions with complex eigenvalues contradicts the behaviour typical of 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 $\gamma_{cr}$. The reason
Figure 6. Wavefunctions for $a = 2.2$ and $g = 0.5$ and values of $\gamma$ close to the exceptional point: ground state (a) and excited state (b) for $\gamma = 0.395$, ground state (c) and excited state (d) for $\gamma = 0.398$. While for $\gamma = 0.395$ small differences can still be recognized, in particular in the imaginary part, the wavefunctions practically coincide at $\gamma = 0.398$.

is that the nonlinear term $g|\Psi|^2$ is a non-analytic 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 $\gamma_c$, 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 $\text{Im}(\Psi(0))$ must also be varied. As a result we find two more complex conjugate solutions that emerge from the coalescing states, see figure 7. The real and imaginary parts of the eigenfunctions and their moduli are shown in figure 8. Obviously the states are not $\mathcal{PT}$ symmetric, and no longer possess vanishing imaginary part at the origin.

2.2.5. Temporal evolution. We finally take a look at the time evolution of a superposition of the two stationary eigenstates in the $\mathcal{PT}$-symmetric regime. While the time dependence of each individual state is given by $\exp(i\kappa^2 t)$, the time evolution of a superposition can no longer be obtained by simply multiplying the individual states by their time evolution factors. The reason is again that the nonlinear term in the Gross–Pitaevskii equation becomes time dependent, and therefore to determine the temporal evolution of an initial superposition the time-dependent Gross–Pitaevskii equation has to be solved. We have done this numerically by applying the split-operator technique, where in the short-time approximation the time evolution operator can be split into products of exponentials of the kinetic and potential terms of the
Figure 7. Eigenvalues of the nonlinear Hamiltonian with $a = 2.2$ for $g = 0.5$ including the analytical continuation as functions of the loss/gain parameter: (a) real part, (b) imaginary part of $\kappa$ (unless zero). Now a pair of complex conjugate eigenvalues also emerges at the exceptional point.

Figure 8. Wavefunctions of the eigenstates of the nonlinear Hamiltonian belonging to the complex eigenvalues of the analytical continuation for $g = 0.5$ and $a = 2.2$ and a loss/gain parameter of $\gamma = 0.5$. The eigenfunctions are not $\mathcal{PT}$ symmetric. The black dotted lines have been drawn to illustrate that $\text{Im}(\Psi_1(x)) \neq 0$.

(nonlinear, time-dependent) Hamiltonian, and the time evolution is calculated by evaluating in every time step the propagator of the kinetic energy term in momentum space and that of the potential energy terms in position space.

In figure 9, we show the results for the time evolution of $|\Psi(x, t)|^2$ of the initial superposition of the ground and the excited state $\Psi(x, 0) = (\psi_1(x) + \psi_2(x))/\sqrt{2}$, for the
nonlinearity \( g = 0.5 \) and different values of the loss/gain parameter. It can be seen that, even with the nonlinearity present, for small \( \gamma \) we have the behaviour typical of \( \mathcal{PT} \)-symmetric systems, i.e. the decrease of the beat length as the loss and gain parameter is growing and the appearance of time intervals in which the probability density in both wells is simultaneously large, or almost completely extinguished.

In figure 9(d), for the value of \( \gamma = 0.3 \) the \( \mathcal{PT} \) symmetry is obviously broken: even though we start with a high probability density in the well with loss, as time proceeds there is no beating, and the well with gain wins. Note that this value of \( \gamma \) is smaller than the value of \( \gamma \approx 0.38 \) where the two complex eigenvalues bifurcate from the ground state branch and smaller than the critical value \( \gamma_c \approx 0.4 \) where the two states coalesce. The reason is that the norm of the state constantly varies with time, and with it the size of the nonlinear term in the Gross–Pitaevskii equation. This effectively corresponds to a variation of \( g \) in the stationary Gross–Pitaevskii equation, and acts as if one were constantly moving through different eigenvalue diagrams. Therefore for a given value of \( g \), the transition to the \( \mathcal{PT} \)-broken phase of the condensate can set in at values of \( \gamma \) smaller than those of the bifurcation and the exceptional point for that value of \( g \).

3. Conclusions and outlook

We have analysed the simple quantum mechanical model of a Bose–Einstein condensate in \( \mathcal{PT} \)-symmetric delta-function double traps by solving the stationary Gross–Pitaevskii equation
first for negligible nonlinearity and then for finite nonlinearity. For vanishing nonlinearity, we find that the eigenvalues and eigenstates exhibit the same behaviour as in an analogous optical system of two $\mathcal{PT}$-symmetric coupled waveguides studied by Klaiman et al [4]. There exist two eigenvalues which merge at a critical value of the loss/gain parameter in a branch point, up to the branch point the corresponding two eigenstates are $\mathcal{PT}$ symmetric, they coalesce at the branch point, beyond the branch point the eigenvalues become complex conjugate, and the $\mathcal{PT}$ symmetry of the wavefunctions is broken.

For finite nonlinearity, we also find two branches of real eigenvalues that merge at an exceptional point. We have the important result that the wavefunctions of the stationary states remain $\mathcal{PT}$ symmetric even if the nonlinearity is present. As a consequence their moduli are even functions, and therefore the nonlinear state-dependent Hamiltonian selects as solutions exactly such states which make the Hamiltonian $\mathcal{PT}$ symmetric. We also find a branch of two complex conjugate eigenvalues for which the $\mathcal{PT}$ symmetry of the wavefunctions is broken.

A surprising result is that, with the nonlinearity present, the branches of complex conjugate eigenvalues do not bifurcate from the exceptional point, but emerge at a smaller value of the loss/gain parameter from the eigenvalue branch of the ground state. This implies that there exist ranges of the loss/gain parameter where four eigenstates exist. This change in the branching scheme of a $\mathcal{PT}$-symmetric nonlinear system is in agreement with the results found by Graefe et al [7] in their investigations of a Bose–Hubbard dimer.

The puzzle that at the exceptional point no branches of complex eigenvalues are born could be solved by analytically continuing the nonlinear term in the Gross–Pitaevskii equation, and we could show that indeed two more complex conjugate solutions are born at this point.

The temporal evolution of an initial superposition of the two stationary states shows, even for non-vanishing nonlinearity, the typical beating patterns known from $\mathcal{PT}$-symmetric systems; but we have found that the breakdown of $\mathcal{PT}$ symmetry occurs at values of the loss/gain parameter smaller than those values where the two branches of complex conjugate eigenvalues bifurcate from the ground state or where the exceptional point appears. This is due to the time variation of the nonlinear term in the Gross–Pitaevskii equation.

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

Our investigations can be extended in several directions. First it will be a worthwhile enterprise to investigate $\mathcal{PT}$-symmetric Bose–Einstein condensates in realistic double-well potentials [26], in one or more dimensions, and possibly pin down physical parameters where the breaking of $\mathcal{PT}$ symmetry could be observed in a real experiment. Also, in addition to the nonlinearity resulting from the short-range contact interaction, condensates with a long-range dipole–dipole interaction [27] could be considered. It would also be interesting whether for the nonlinear $\mathcal{PT}$-symmetric Hamiltonian considered in this paper, similar to the work of Jones [12], the construction of a metric operator is possible with respect to which the nonlinear Hamiltonian is quasi-Hermitian. Furthermore it would be desirable to find simple matrix models which show the unusual branching scheme of the eigenvalues found for finite nonlinearity.

Acknowledgment

We thank Eva-Maria Graefe and Miloslav Znojil for helpful comments.
Appendix. The Gross–Pitaevskii equation

Expressed in terms of physical quantities, the Gross–Pitaevskii equation for a condensate in a $\mathcal{PT}$-symmetric delta-function double well reads

$$
-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x) - \left[ (V_0 + i\Gamma) \delta(x + b) + (V_0 - i\Gamma) \delta(x - b) - G|\Psi(x)|^2 \right] \Psi(x) = \mu \Psi(x).
$$

(A.1)

The depths of the double well are determined by $V_0$, the size of the gain and loss terms by $\pm \Gamma$. The amplitude of the nonlinear term which arises from the contact interaction between the condensate atoms is given by the quantity $G$ and is proportional to the scattering length of the condensate atoms, $\mu$ is the chemical potential. Measuring lengths in units of $L = \hbar^2/(2mV_0)$ and energies in units of $E_0 = 2mV_0^2/\hbar^2$ brings (A.1) into the dimensionless form given in (1).

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