Description of Bose-Einstein condensates in $\mathcal{PT}$-symmetric double wells

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Abstract. The Gross-Pitaevskii equation for a Bose-Einstein condensate in a $\mathcal{PT}$-symmetric double-well potential is investigated theoretically. An in- and outcoupling of atoms is modelled by an antisymmetric imaginary potential rendering the Hamiltonian non-Hermitian. Stationary states with real energies and $\mathcal{PT}$-symmetric wave functions are found, which proves that Bose-Einstein condensates are a good candidate for a first experimental verification of a $\mathcal{PT}$-symmetric quantum system. Time-resolved calculations demonstrate typical effects only observable in $\mathcal{PT}$-symmetric potentials, viz. an oscillation of the condensate's probability density between these wells with an oscillation frequency critically depending on the strength of the in- and outcoupling. $\mathcal{PT}$-broken eigenstates with complex energy eigenvalues are also solutions of the time-independent Gross-Pitaevskii equation but are not true stationary states of its time-dependent counterpart. The comparison of a one-dimensional and a three-dimensional calculation shows that it is possible to extract highly precise quantitative results for a fully three-dimensional physical setup from a simple one-dimensional description.

Keywords: Bose-Einstein condensates, $\mathcal{PT}$ symmetry, Gross-Pitaevskii equation, stationary states, dynamics

1 Introduction

Mainly due to the experimental accessibility, which became possible very recently [1, 2], non-Hermitian $\mathcal{PT}$-symmetric quantum mechanics has gained an increasing attention over the last years [1–17]. It describes physical systems governed by a complex Hamiltonian which is not Hermitian but fulfils parity-time symmetry. This means that the Hamiltonian remains invariant under the combined action of the parity ($\mathcal{P}$) and time reversal ($\mathcal{T}$) operators, i.e. $[\mathcal{PT}, H] = 0$, with

$$\mathcal{P}x = -x\,, \qquad \mathcal{P}p = -p \tag{1a}$$

$$\mathcal{T}x = x\,, \qquad \mathcal{T}p = -p\,, \qquad \mathcal{T}\mathrm{i} = -\mathrm{i}\,. \tag{1b}$$

In spite of their non-Hermiticity these Hamiltonians possess real energy spectra for properly chosen physical parameters. Besides the emergence of real energy eigenvalues, phenomena are observable which are only possible in non-Hermitian systems and not known in Hermitian quantum mechanics describing the spectra of bound states. The most striking effects are connected with so-called exceptional points [18], i.e. isolated points in the physical parameter space at which two or even more solutions pass through a branch point singularity, where both the energies *and* the wave functions of the two states become identical.

Bender and Boettcher introduced a simple and instructive model that covers all interesting features of a $\mathcal{PT}$-symmetric quantum system [3]. It consists of the Hamiltonian

$$H = p^2 - (\mathrm{i}x)^N \,, \tag{2}$$

where N is allowed to assume the value of any real number. In a very simple calculation it can be confirmed that $[\mathcal{PT}, H] = 0$, i.e. this Hamiltonian is $\mathcal{PT}$ symmetric. Evidently, $N = 2$ represents the harmonic oscillator, of which we know that its spectrum is real and positive. Bender and Boettcher found that this fact remains true for all $N \geq 2$, however, if N is reduced below 2 one observes that successively one pair of consecutive eigenvalues after the other passes through a branch point singularity. Beyond the branch point both eigenvalues become complex and complex conjugate. This eigenvalue structure already describes the typical behaviour of parameter-dependent $\mathcal{PT}$-symmetric Hamiltonians.

In the wake of the discovery of Bender and Boettcher, a large number of systems with $\mathcal{PT}$-symmetric Hamiltonians have become the subject of theoretical and experimental studies. It is no surprise that the most sophisticated experimental progress in the investigation of $\mathcal{PT}$-symmetric physical systems has been achieved in optics [5, 7, 9, 12, 15, 16, 19]. The gain and loss contributions required to set up a non-Hermitian $\mathcal{PT}$-symmetric system can be implemented, e.g. with optical pumping (gain) and absorptive media (loss), i.e. by exploiting well established techniques.

Due to the well known analogy that the wave equation for the transverse electric field mode is formally equivalent to a one-dimensional Schrödinger equation these optical systems can be considered as a simulation of the motion of a quantum particle in a potential of the form $V(x) = -k^2 n^2(x)$, where n is the (complex) refractive index. However, these studies cannot completely substitute studies of quantum systems, and the verification of $\mathcal{PT}$ symmetry in a true quantum system is highly desirable. Klaiman et al. [9] proposed a quantum analogue to the optical experiments consisting of a Bose-Einstein condensate in a double-well potential. The gain and loss terms could be realised by coherently removing atoms from one well and injecting atoms into the other.

At sufficiently low temperatures one may assume that *all* atoms of a dilute gas of weakly interacting Bosons trapped in an optical potential are in their ground state. Then the system can be well described by the Gross-Pitaevskii equation [20, 21], i.e. the Hartree approximation of the corresponding many-particle equation, where all single-particle orbitals are given by the same state. In a particle number scaled form and in appropriate units the Gross-Pitaevskii

equation reads

$$\mathrm{i}\dot{\psi}(\boldsymbol{x},t) = \left(-\Delta + V(\boldsymbol{x}) - g|\psi(\boldsymbol{x},t)|^2\right)\psi(\boldsymbol{x},t)\ . \tag{3}$$

The trapping potential for the atoms is described by $V(\boldsymbol{x})$. Additionally, the atoms interact via the short-range van der Waals force, of which a description with an s-wave scattering process is sufficient in the dilute gas. Its strength g is determined by the scattering length.

It is the scattering term $-g|\psi(\boldsymbol{x},t)|^2$ which needs a further consideration since it leads to a crucial modification of the Schrödinger equation. The Gross-Pitaevskii equation (3) is nonlinear in the wave function. This has direct consequences for the $\mathcal{PT}$ symmetry of the system. For a $\mathcal{PT}$-symmetric system we require, as mentioned above, $[\mathcal{PT}, H] = 0$. Since the kinetic energy term in the Hamiltonian is always $\mathcal{PT}$ symmetric one directly obtains the necessary condition for the potential,

$$V^*(-\boldsymbol{x}) = V(\boldsymbol{x})\ . \tag{4}$$

This has also to be fulfilled by the scattering term. Thus, for the total Hamiltonian to be $\mathcal{PT}$ symmetric the square modulus of the wave function which is the solution of the Gross-Pitaevskii equation has to be a symmetric function of $\boldsymbol{x}$.

In previous studies of $\mathcal{PT}$-symmetric systems with nonlinearity it was found that the nonlinearity not necessarily destroys the appearance of real eigenvalues in the spectrum or their coalescence in branch point singularities. Indeed, $\mathcal{PT}$-symmetric eigenstates with real energies have been found for a non-Hermitian Bose-Hubbard model [10, 11, 22], quantum mechanical model potentials [8], optical waveguide structures [7, 15], and for Bose-Einstein condensate in an idealised double-δ trap [23, 24], or in a spatially extended double well [25].

In this article we will solve the Gross-Pitaevskii equation for a Bose-Einstein condensate in a double well with antisymmetric imaginary potential contributions describing effectively gain and loss processes. We show that it exhibits $\mathcal{PT}$-symmetric solutions, which is important because $\mathcal{PT}$-symmetric wave functions always have a square modulus which is a symmetric function of the coordinate x. A Bose-Einstein condensate is a fully three-dimensional object, however, for the investigation of the $\mathcal{PT}$ symmetry only a gain-loss profile in one spatial direction is required. Thus, one may assume that it is sufficient to reduce the theoretical description to one dimension without losing any relevant information. We will demonstrate that this is exactly the case. But the correspondence of the one- and three-dimensional solutions we obtain is even stronger. We show that the solution of a Gross-Pitaevskii equation with adequately rescaled nonlinearity is capable of providing quantitatively correct predictions for the fully three-dimensional treatment. By the variation of the trap frequencies it will always be possible to realise a regime in which the influence of the two additional dimensions can be obtained without any explicit calculation. Furthermore, we show that a stable dynamics of condensate wave functions is possible in the system with gain and loss. This will be crucial for an experimental observability.

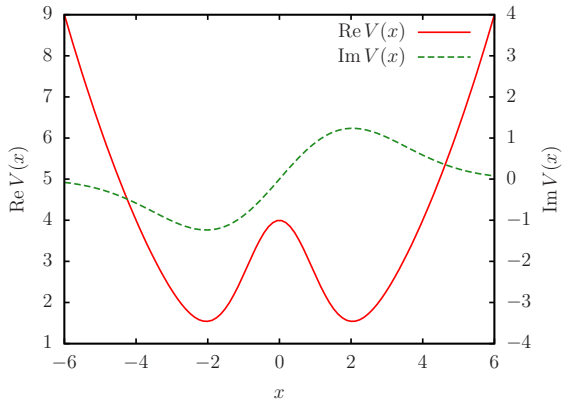

Fig. 1. Visualisation of the $\mathcal{PT}$-symmetric external potential in x direction. The real part (solid line) defines the confinement of the condensed atom cloud, and the imaginary part (dashed line) describes the in-/outcoupling of atoms.

In Sect. 2 we present the system and the corresponding Gross-Pitaevskii equation. Additionally, we introduce two numerical methods for the calculation of the stationary states. Then we discuss the numerical results for the energy eigenvalues and investigate quantitatively the quality of one-dimensional model calculations for the fully three-dimensional condensate in Sect. 3. Finally, we study the stability of the condensate with numerically accurate dynamical computations in Sect. 4. Conclusions are drawn in Sect. 5.

2 Theoretical description of the Bose-Einstein condensate in the double well

2.1 Gross-Pitaevskii equation

The Bose-Einstein condensate of atoms with mass m is, in the mean-field limit, described by the Gross-Pitaevskii equation (3), where we assume a potential of the form

$$V(\boldsymbol{x}) = \frac{m}{2}\omega_x^2 x^2 + \frac{m}{2}\omega_{y,z}^2(y^2+z^2) + v_0 e^{-\sigma x^2} + \mathrm{i}\Gamma x \mathrm{e}^{-\rho x^2} \ . \tag{5}$$

It consists of a three-dimensional harmonic trap with trapping frequencies ω_x for the x direction and $\omega_{y,z}$ for the two remaining spatial coordinates. To form a double well it is superimposed with a Gaussian barrier in x direction. This results in the one-dimensional projection of the potential as shown in Fig. 1. It is obvious that the barrier has its maximum at $x = 0$. Its height is v_0 and the width of the Gaussian is given by σ. The imaginary contribution of strength Γ is an effective description of a gain or loss of atoms. As can be confirmed by a simple calculation the external potential (5) is $\mathcal{PT}$ symmetric.

The coherent addition and removal of atoms proposed by Klaiman et al. [9] can in principle be achieved by several methods. For example, appropriate laser setups forming Bragg beams may be exploited to actively transport atoms from a reservoir to one of the wells and to eject atoms from the other [26, 27]. The reservoir can be a third well or a completely independent trap geometry. One may also imagine a geometry with multiple wells in a row. If these wells are close enough such that the condensate's probability density may tunnel from one well to its neighbouring well a flow of particles with a defined direction could be generated by different potential offsets for the single wells. However, in this article we concentrate on the effects of the $\mathcal{PT}$-symmetric external potential and will keep the equations as simple as possible. Thus, we adopt the formalism used for the optical systems [5, 7, 9, 12, 15, 16, 19], where a complex refractive index was used, and simulate an outcoupling of atoms with a negative imaginary potential contribution in the left well, whereas a positive imaginary part in the right well reflects in incoupling of atoms. Since the potential affects the probability amplitude of the whole condensate the physical interpretation is a *coherent* coupling, which is in agreement with our physical interpretation of the process since we do not consider individual atoms but a macroscopic wave function of the condensed phase.

With the length scale $a_0 = \sqrt{\hbar/2m\omega_x}$ defined by the trap frequency in the direction of the double well and the unit of energy $E_0 = \hbar^2/2ma_0^2$ the dimensionless potential assumes the form

$$V(\boldsymbol{x}) = \frac{1}{4}x^2 + \frac{1}{4}\omega_{y,z}^2(y^2+z^2) + v_0 e^{-\sigma x^2} + \mathrm{i}\Gamma x \mathrm{e}^{-\rho x^2} \ . \tag{6}$$

Then the dynamics is governed by the time-dependent Gross-Pitaevskii equation (3). To obtain stationary solutions we solve its time-independent variant, viz.

$$\left(-\Delta + V(\boldsymbol{x}) - g|\phi(\boldsymbol{x})|^2\right)\phi(\boldsymbol{x}) = \mu\phi(\boldsymbol{x}) \ , \tag{7}$$

where the chemical potential μ has been introduced with the usual ansatz $\psi(\boldsymbol{x},t) = \phi(\boldsymbol{x})\mathrm{e}^{-\mathrm{i}\mu t}$. For all calculations we keep the parameters $v_0 = 4$ and $\sigma = 0.5$ fixed. The width parameter ρ of the imaginary gain-loss potential is chosen to be

$$\rho = \frac{\sigma}{2\ln(4v_0\sigma)} \ . \tag{8}$$

This choice guarantees that the extrema of the real and imaginary potential parts coincide, as is illustrated in Fig. 1. A one-dimensional description is obtained with the potential

$$V(x) = \frac{1}{4}x^2 + v_0 e^{-\sigma x^2} + \mathrm{i}\Gamma x \mathrm{e}^{-\rho x^2} \ , \tag{9}$$

in which only the x direction is considered and all y and z terms are removed. Obviously it contains all the relevant information about the $\mathcal{PT}$ symmetry.

2.2 Numerical methods

We apply two independent methods to solve the time-dependent and time-independent Gross-Pitaevskii equations (3) and (7). Our first method is a Gaussian variational approach [28, 29] based on the idea to restrict the wave function to a Gaussian form, viz.

$$\psi(\boldsymbol{z},\boldsymbol{x}) = \sum_{k=1}^{N_\mathrm{G}} \mathrm{e}^{-\left[A_x^k (x-q_x^k)^2 + A_{y,z}^k (y^2+z^2)\right]} \mathrm{e}^{\mathrm{i}p_x^k (x-q_x^k) - \varphi^k} \ . \tag{10}$$

Within this approach the dynamics is described by the small set of variational parameters

$$\boldsymbol{z}(t) = \left\{ A_x^k(t), A_{y,z}^k(t), q_x^k(t), p_x^k(t), \varphi^k \right\} \ . \tag{11}$$

The most simple ansatz is a superposition of two Gaussian wave functions, each of them located in one of the wells, i.e. $N_\mathrm{G} = 2$ in (10). Then the real coordinates q_x^1, q_x^2, p_x^1 and p_x^2 determine the positions and momenta of the Gaussians. The widths of the Gaussians are given by the complex parameters A_x^1, A_x^2, $A_{y,z}^1$ and $A_{y,z}^2$, where we chose identical widths for the y and z directions, in agreement with the symmetry of the external potential (5). Finally, the complex quantities φ^1 and φ^2 determine the amplitudes and phases.

The application of the McLachlan time-dependent variational principle [30],

$$\delta I = \delta || i\chi(\boldsymbol{z}(t),\boldsymbol{x}) - H\psi(\boldsymbol{z}(t),\boldsymbol{x})||^2 \stackrel{!}{=} 0 \ , \tag{12}$$

leads to a set of ordinary differential equations for the parameters (11) after the variation with respect to χ and the subsequent replacement $\dot{\psi} \equiv \chi$. Stationary states or solutions of the time-independent Gross-Pitaevskii equation (7) are found if the conditions $\dot{A}_x^k = \dot{A}_{y,z}^k = \dot{q}_x^k = \dot{p}_x^k = 0$, and $\dot{\varphi}^1 = \dot{\varphi}^2$ are fulfilled. A detailed explanation of the procedure can be found in reference [25].

The advantage of the Gaussian variational method is its high scalability, i.e. the difference of the numerical costs between the one- and three-dimensional descriptions is very moderate. Nevertheless, it provides highly precise solutions [31–33]. However, since in this analysis of $\mathcal{PT}$-symmetric Bose-Einstein condensates the method is applied for the first time to nonlinear complex potentials we compare its results to numerically exact solutions of the Gross-Pitaevskii equation in one dimension. To obtain the numerically exact stationary states the wave functions are integrated outward from $x = 0$ in positive and negative direction using a Runge-Kutta algorithm. The initial values $\mathrm{Re}\,\psi(0), \psi'(0) \in \mathbb{C}$, and $\mu \in \mathbb{C}$ are chosen such that the wave functions are square integrable ($\psi(\infty) \to 0, \quad \psi(-\infty) \to 0$) and normalised $||\psi|| = 1$. For numerically exact dynamical calculations we apply the split-operator method.

3 Stationary states

3.1 General behaviour of the solutions

Fig. 2 shows the results of the solution of the Gross-Pitaevskii equation (7). Let

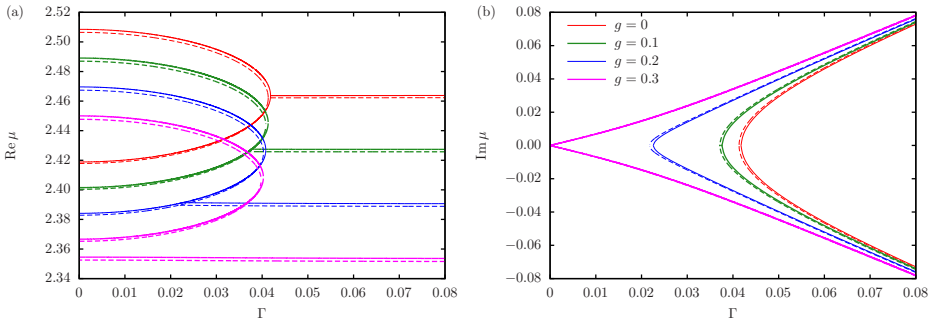

Fig. 2. Real and imaginary parts of the energy eigenvalues μ of the stationary Gross-Pitaevskii equation (7) as a function of the the gain-loss parameter Γ. The Gaussian approximation (solid lines) and the numerically exact solutions (dashed lines) show an excellent agreement. In the left panel, g increases from top to bottom, in the right panel from right to left.

us first concentrate on the linear case $g = 0$, which exhibits the typical behaviour known from other $\mathcal{PT}$-symmetric systems (top curve in the left panel and rightmost curve in the right panel). Below a critical value $\Gamma_{\mathrm{EP}} \approx 0.04$ of the gain-loss parameter Γ we find two real eigenvalues, corresponding to a ground state with completely symmetric wave function for $\Gamma = 0$ and an excited state, of which the wave function is completely antisymmetric for $\Gamma = 0$. At $\Gamma_{\mathrm{EP}} \approx 0.04$ the two solutions merge in an exceptional point, where we have confirmed that indeed the wave functions become identical. Increasing Γ further we obtain two complex conjugate solutions. One also notes that the agreement between the Gaussian approximation and the numerically exact solution is excellent.

Obviously the real eigenvalues do not vanish in the case $g \neq 0$. This is an important result since it indicates a persistence of the $\mathcal{PT}$ symmetry in the nonlinear quantum system. Non-decaying states are present. However, if we want to be sure about the symmetry we have to look at the wave functions. As mentioned in the introduction the $\mathcal{PT}$ symmetry of the Gross-Pitaevskii equation (7) depends on its solution, or, to be more precise, on the shape of the wave function's square modulus. It has to be a symmetric function of x. Is this the case? The answer to this question is given in Figs. 3(a) and (b), which show the wave functions belonging to both real eigenvalues for $g = 0.2$ and $\Gamma = 0.03$. The square moduli are symmetric functions of x. This confirms that the case of exact $\mathcal{PT}$ symmetry is fulfilled.

There are also, as in the linear case, states with complex eigenvalues. From linear $\mathcal{PT}$-symmetric models we know that these complex eigenvalue solutions belong to $\mathcal{PT}$-broken wave functions. This behaviour is also found in our case, cf. Figs. 3(c) and (d). This has crucial impact on the nonlinear Gross-Pitaevskii equation. Since the square moduli of the wave functions are not symmetric functions of x the $\mathcal{PT}$ symmetry of the *Hamiltonian* is destroyed.

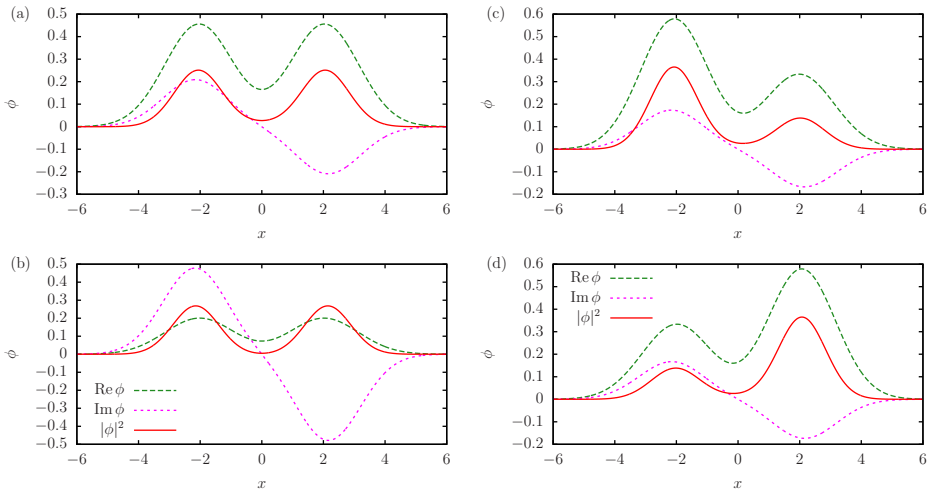

Fig. 3. The wave functions of the ground (a) and the excited (b) eigenstates with real eigenvalues possess symmetric square moduli, and thus correspond to the case of exact $\mathcal{PT}$ symmetry. By contrast, the wave functions of the complex eigenvalue solutions with negative (c) and positive (d) imaginary part do not have symmetric square moduli. All wave functions are shown for $g = 0.2$ and $\Gamma = 0.03$. Since there are almost no visible differences between the variational Gaussian and the numerically exact solutions only the variational wave functions are drawn.

In Fig. 2 we observe a further crucial difference between the linear and the nonlinear system. In the linear case $g = 0$ the two complex eigenvalue solutions emerge exactly at the value Γ_{EP} at which the non-decaying eigenstates with real eigenvalues vanish. This does not hold for the nonlinear system, i.e. for $g \neq 0$. In the latter case the complex eigenvalue solutions are born at a value $\Gamma_{\mathrm{c}} < \Gamma_{\mathrm{EP}}$. At the exceptional point Γ_{EP} only the real eigenvalue states vanish and new complex solutions do not appear. It is known that this unusual bifurcation scenario has its origin in the non-analyticity of the Gross-Pitaevskii equation [25, 34], which is a topic of ongoing research.

3.2 Importance of the one-dimensional solutions

Since only the x coordinate is relevant for the $\mathcal{PT}$ symmetry of the potential (5) it is not surprising that the one-dimensional calculations considered so far already cover qualitatively all relevant effects. However, we want to go one step further and ask whether the one-dimensional calculations are also capable of providing precise quantitative predictions for a completely three-dimensional setup. To do so, we investigate simple but plausible assumptions on the two remaining directions and their influence on the energy eigenvalues.

The first effect of the two additional directions is clearly the interaction of the atoms in the condensate with the trapping potentials defined by the trap frequency $\omega_{y,z}$ in (6). If we assume that only the ground state of the corresponding

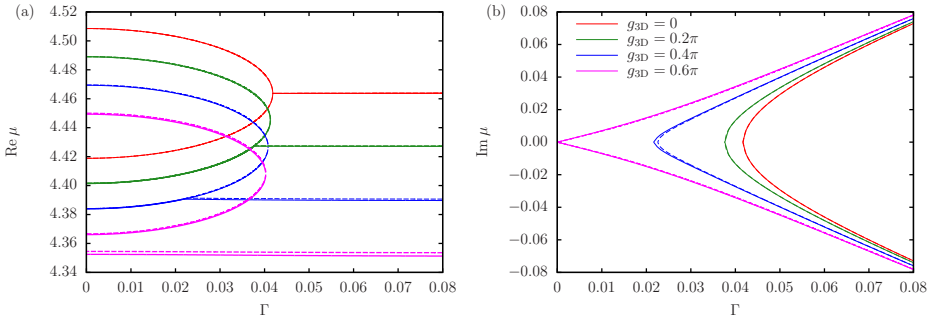

Fig. 4. The real (a) and nonvanishing imaginary (b) parts of the energy eigenvalues of the one-dimensional model (dashed lines) are compared with the fully three-dimensional calculations (solid lines). One observes a very good quantitative description by the simple one-dimensional treatment of the system. The differences can hardly be seen in the graph. Again, in the left panel, g increases from top to bottom, and in the right panel from right to left.

oscillators is occupied, which is reasonable in the condensed phase, we obtain an energy shift by a value of $\Delta\mu = \omega_{y,z} = 2$ in the units introduced in Sect. 2.1.

Since the Gross-Pitaevskii equation (7) contains also the nonlinear scattering term we have to take into account the normalisation integral for the energy contribution of the s-wave contact interaction. An estimate of the difference between the one- and three-dimensional contact energies can be extracted from its expectation value. We wish to describe the three-dimensional setup by an equivalent one-dimensional model, and thus we demand that the expectation values of both contact energies are identical, viz.

$$\int_{\mathbb{R}^3} dx\, dy\, dz\, g_{3\mathrm{D}} |\psi_{3\mathrm{D}}(\boldsymbol{x})|^4 \stackrel{!}{=} \int_{\mathbb{R}} dx\, g_{1\mathrm{D}} |\psi_{1\mathrm{D}}(x)|^4 \,. \tag{13}$$

This leads to the relation

$$g_{3\mathrm{D}} = \frac{4\pi}{\omega_{y,z}} g_{1\mathrm{D}} \tag{14}$$

between the value $g_{1\mathrm{D}}$ which has to be used in the one-dimensional model in order that it results in the same contact energy as a three-dimensional wave function with $g_{3\mathrm{D}}$. Again, we assumed that the harmonic oscillator ground state with its wave function ψ_0 is a good approximation for the directions y and z. Furthermore, we used the product ansatz

$$\psi_{3\mathrm{D}}(\boldsymbol{x}) \approx \psi_{1D}(x)\psi_0(y)\psi_0(z) \,. \tag{15}$$

Of course, these simple considerations are only correct in the linear form of the Gross-Pitaevskii equation (7), with $g = 0$. However, in Fig. 4 we observe a remarkable agreement between the one-dimensional results based on the simple assumptions and the results of the fully three-dimensional calculations even

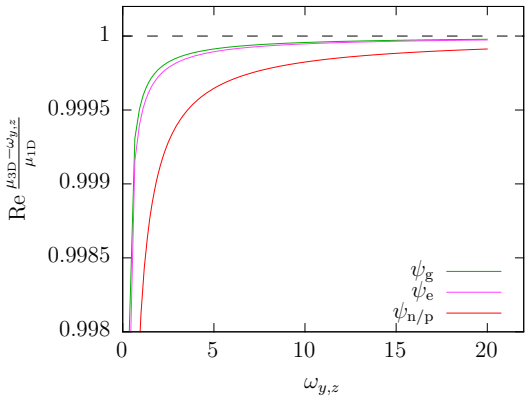

Fig. 5. Real part of the ratio (16) as a function of $\omega_{y,z}$ for the ground state ψ_g, the excited state ψ_e, and the $\mathcal{PT}$-broken states $\psi_{n/p}$. All calculations are carried out for a nonlinearity of $g_{3D} = 1.2\pi/\omega_{y,z}$, i.e. $g_{1D} = 0.3$. For higher values of $\omega_{y,z}$ the ratio converges to unity, i. e. the agreement between the solutions in one and three dimensions becomes better and better. The $\mathcal{PT}$-symmetric solutions converge faster than the $\mathcal{PT}$-broken solutions.

for nonlinearities as large as $g_{1D} \approx 0.3$. It is almost impossible to identify the differences.

In a further step one may assume that the one-dimensional description even becomes better when the geometry of the setup is designed to favour the spatial extension in only the x direction. The previous calculations for the three-dimensional potential were carried out with a constant trapping frequency of $\omega_{y,z} = 2$. The trapping frequencies influence the condensate's shape, and thus it is expected that they have an impact on how precise the stationary solutions in one dimension can be transferred to solutions in three dimensions. The limit $\omega_{y,z} \to \infty$ effectively describes the one-dimensional potential because the widths of the wave function in y and z directions must vanish. Therefore the behaviour in the three-dimensional potential can be predicted more accurately by the one-dimensional solutions for higher values of $\omega_{y,z}$. Figure 5 confirms the convergence of the energy eigenvalues in the three-dimensional potential to the solutions in one dimension with increasing $\omega_{y,z}$. What is shown is the value of the ratio

$$\frac{\mu_{3D} - \Delta\mu}{\mu_{1D}} = \frac{\mu_{3D} - \omega_{y,z}}{\mu_{1D}}. \tag{16}$$

If the solutions in three dimensions are exactly described by the product ansatz (15) the ratio will be equal to one. Indeed, we observe convergence to unity for increasing values of $\omega_{y,z}$.

The convergence in the limit $\omega_{y,z} \to \infty$ is expected. What is, however, of greater interest is, at which values of the trapping frequencies the one-dimensional model becomes sufficiently accurate. We see from Figure 5 that in particular for

the stationary solutions with real eigenvalues, i.e. the $\mathcal{PT}$-symmetric states, one has rapid convergence. To achieve a good agreement between the solutions in one and three dimensions it is obviously sufficient to choose a trapping frequency $\omega_{y,z}$ which is larger than that for the x direction, i.e. in the units used for our calculation $\omega_{y,z} > 1$. This is remarkable since this does by far not mean that we are investigating a quasi one-dimensional setup. The spatial extension in y and z directions may be comparable to that in x direction and it is still possible to extract quantitatively correct values from a simple and numerically less expensive one-dimensional calculation.

4 Dynamics of the condensate

Before we investigate the temporal evolution of the wave functions we have to note an important consequence of the nonlinear system with gain and loss. In Sect. 3.1 we observed $\mathcal{PT}$-broken solutions with complex energy eigenvalues and called them stationary states. From the point of view of the time-dependent Gross-Pitaevskii equation (3) this is not correct. The consequence of the imaginary parts of the energies is a decay or growth of the state's probability amplitude. This affects the scattering term $-g|\psi|^2$, and introduces an explicit time dependence into the nonlinear Hamiltonian. Thus, these states cannot be considered to be true stationary solutions of the time-dependent Gross-Pitaevskii equation. Strictly speaking, they lose their physical relevance. We will see, however, that they still have important consequences for the dynamics of the whole system.

If we prepare the condensate in a state close to the stationary real eigenvalue solutions for values of Γ below the appearance of the $\mathcal{PT}$-broken states their influence is supposed to be negligible. This can be confirmed in a numerically exact propagation of such initial states using the split-operator method. Since we have demonstrated in Sect. 3.2 that a fully three-dimensional calculation is not necessary we restrict our calculations to the one-dimensional model which is more illustrative.

In Figs. 6(a), (b), and (c) we visualise the evolution of the probability amplitude of an initial wave packet

$$\psi(x, t = 0) = \frac{1}{\sqrt{2}} \left(\phi_{\mathrm{g}}(x) + \mathrm{e}^{\mathrm{i}\varphi} \phi_{\mathrm{e}}(x) \right) \ , \tag{17}$$

where $\phi_{\mathrm{g}}(x)$ and $\phi_{\mathrm{e}}(x)$ are the ground and excited state, respectively, and $\varphi = \pi/2$ was chosen. We observe the same behaviour as it appears already in linear systems [9]. An oscillation of the probability amplitude between the two wells sets in, and the oscillation frequency decreases with increasing Γ. Close to the exceptional point at $\Gamma \approx 0.04$ the oscillation period tends to infinity. A detailed quantitative analysis reveals that the influence of the nonlinearity is only a slightly higher oscillation frequency as compared to the linear case $\Gamma = 0$.

A drastic qualitative change of the wave function's behaviour is observed in Fig. 6(d), where the phase was chosen to be $\varphi = \pi$ and the gain-loss parameter

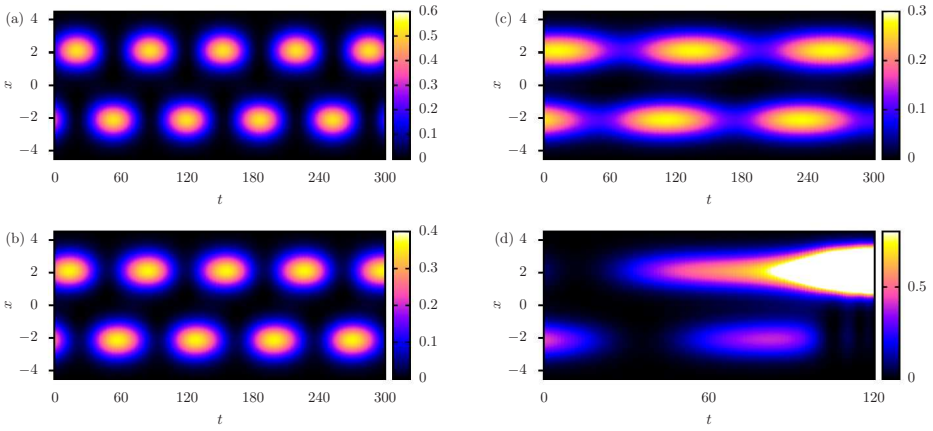

Fig. 6. Visualisation of the probability amplitude's spatial distribution as a function of time. The initial wave packet is defined by (17). In all calculations $g = 0.2$ was chosen. For the choice $\varphi = \pi/2$ stable oscillations are observable in the cases $\Gamma = 0$ (a), $\Gamma = 0.02$ (b), and $\Gamma = 0.04$ (c). For $\Gamma = 0.03$ and $\varphi = \pi$ we observe an explosion of the wave packet (d).

$\Gamma = 0.03$ is in a regime in which the additional $\mathcal{PT}$-broken states are present for $g = 0.2$, cf. Fig. 2. The condensate does not oscillate between the wells. The probability amplitude tunnels into the well with gain ($x > 0$) which leads immediately to an "explosion" of the wave function, i.e. it grows beyond all limits. Of course this is only correct in our description of the gain and loss effects with imaginary potentials which correspond to infinitely large reservoirs. In a realistic situation this description will break down at some point.

There is a simple explanation for the exploding behaviour. The two $\mathcal{PT}$-broken solutions with complex eigenvalues exist and they possess a considerable overlap with the time-evolved wave function (17). In this case the eigenstate with positive imaginary part of the energy can dominate the long-time behaviour since it grows. This can also happen close to the ground state, which does not need to be stable in the nonlinear system with gain and loss. In fact, a detailed stability analysis by solving the Bogoliubov-de Gennes equations confirms that the ground state becomes unstable as soon as the complex eigenvalue solutions emerge at a critical value Γ_c [25].

As we have seen in Fig. 6(c) the instability of the ground state does not necessarily lead immediately to a destruction of the oscillation. For the value $\Gamma = 0.04$, i.e. very close to the exceptional point also the $\mathcal{PT}$-broken solutions exist. However, the probability amplitude almost pulsates in both wells with a low frequency as it is known from linear $\mathcal{PT}$-symmetric systems, and does not seem to be disturbed by the growing and decaying complex eigenvalue solutions. An extensive study of the initial conditions reveals that the phase φ in (17) critically influences the fate of the initial wave packet.

5 Conclusion

The most important result of this work is the verification of the existence of $\mathcal{PT}$-symmetric eigenstates of the Gross-Pitaevskii equation for a Bose-Einstein condensate in an external $\mathcal{PT}$-symmetric potential. Due to an incoupling and outcoupling of atoms in the two wells, which can be described by imaginary potential contributions, the Hamiltonian is complex and non-Hermitian. It does not necessarily need to support true stationary states. However, the $\mathcal{PT}$-symmetric solutions possess real energy eigenvalues, and thus demonstrate that stationary eigenstates that do not decay or grow exist even though a gain and loss of atoms is always present. This behaviour is known from linear $\mathcal{PT}$-symmetric quantum systems, but its appearance in the mean-field description of Bose-Einstein condensates is a nontrivial finding since the Hamiltonian of the Gross-Pitaevskii equation is nonlinear. Thus, the solution has an effect on the Hamiltonian's symmetry, i.e. only after the wave functions have been found one can be sure that the system fulfils any symmetry. In other words, one may conclude that the Hamiltonian picks as real eigenvalue solutions exactly those states which render itself $\mathcal{PT}$ symmetric.

The real energy eigenvalues are the only true stationary states of the system. It is also possible to find solutions of the time-independent Gross-Pitaevskii equation with complex energy eigenvalues. However, they cannot be considered to be physical. Due to the decay or growth enforced by the imaginary energy contributions these states introduce an explicit time dependence into the nonlinear Hamiltonian, and thus are not stationary solutions of the time-dependent Gross-Pitaevskii equation. As is known from linear systems the complex energies found for the time-independent Gross-Pitaevskii equation belong to wave functions with broken $\mathcal{PT}$ symmetry. Since their square moduli are not symmetric functions of the spatial coordinates they destroy also the Hamiltonian's $\mathcal{PT}$ symmetry. A striking difference between linear and nonlinear systems is the point of emergence of the states with broken $\mathcal{PT}$ symmetry. In linear systems they are born exactly at the critical parameter value Γ_{EP} at which the two real eigenvalue states vanish in an exceptional point. For a nonvanishing nonlinearity g we observe that the complex eigenvalue solutions bifurcate from the ground state at a lower gain-loss parameter Γ_c.

It is remarkable that the effects of the $\mathcal{PT}$-symmetric double well can be excellently described by one-dimensional calculations. Of course, one can immediately see that it is possible to construct a one-dimensional $\mathcal{PT}$-symmetric potential. Then one does not expect to lose any qualitative information when one reduces a fully three-dimensional physical system to a one-dimensional description. Our calculations showed that for Bose-Einstein condensates in a double well the correspondence between three- and one-dimensional calculations is even stronger. Highly precise quantitative predictions for the energy eigenvalues of the physical condensate wave function can be obtained from simple one-dimensional considerations. This fact holds for condensate geometries which by far cannot be called one-dimensional.

The time evolution of the wave functions revealed that for low enough gain-loss parameters Γ the condensate behaves as waves in linear $\mathcal{PT}$-symmetric systems. The probability amplitude oscillates between the wells, where the oscillation frequency decreases for increasing Γ and tends to zero close to the exceptional point at which the real eigenvalues solutions merge. As soon as Γ is strong enough for the appearance of the $\mathcal{PT}$-broken complex energy states the temporal evolution of the condensate can become unstable and lead to an infinite growth of the probability amplitude in the well with gain. This effect depends critically on the preparation of the initial state. For an experimental realisation the most important finding is the existence of a stable dynamics.

The present work shows that Bose-Einstein condensates are good candidates for the first experimental observation of a $\mathcal{PT}$-symmetric quantum system. However, there are still some questions which have to be answered. So far, we introduced the coherent in- and outcoupling of atoms only via complex potentials. A topic of ongoing research are several setups with additional wells acting as reservoirs of atoms. These setups are based on the idea that one has a closed system in which the double well is embedded. We wish to investigate how it is possible to drive a coherent flow of atoms between the reservoir and the two wells such that the double well alone can *effectively* be described by the imaginary potential presented in this article.

From the theoretical point of view it would be desirable to understand how a coherent in- or outcoupling of atoms can be understood on a microscopic level. This will require considerations beyond the mean-field limit but will certainly provide more insight into the physical processes. The systems also revealed a number of mathematical challenges. The unusual bifurcation scenario with the $\mathcal{PT}$-symmetric solutions bifurcating from the ground state has its origin in the non-analyticity of the Gross-Pitaevskii equation. The investigation of the nature of these bifurcation points requires a proper analytic extension.

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