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Matter-wave gap solitons and vortices in three-dimensional parity-time-symmetric optical lattices

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SUMMARY

Past decades have witnessed the emergence and increasing expansion of paritytime (\mathcal{PT})-symmetric systems in diverse physical fields and beyond as they manifest entirely all-real spectra, although being non-Hermitian. Nonlinear waves in low-dimensional \mathcal{PT} -symmetric non-Hermitian systems have recently been explored broadly; however, understanding these systems in higher dimensions remains abstruse and has yet to be revealed. We survey, theoretically and numerically, matter-wave nonlinear gap modes of Bose-Einstein condensates with repulsive interparticle interactions in three-dimensional \mathcal{PT} optical lattices with emphasis on multidimensional gap solitons and vortices. Utilizing direct perturbed simulations, we address the stability and instability areas of both localized modes in the underlying linear band gap spectra. Our study provides deep and consistent understandings of the formation, structural property, and dynamics of coherent localized matter waves supported by \mathcal{PT} optical lattices in multidimensional space, thus opening a way for exploring and stabilizing three-dimensional localized gap modes in non-Hermitian systems

INTRODUCTION

Stabilizing multidimensional localized modes is challenging in attractive nonlinear Kerr media, as the catastrophic self-focusing nonlinearity poses a serious problem of critical and supercritical wave collapse (or blowup), respectively, in two- (2D) and three-dimensional (3D) free space (Chiao et al., 1964; Bergé, 1998; Sulem and Sulem, 1999; Kivshar and Pelinovsky, 2000; Lederer et al., 2008; Chen and Hung, 2021; Zeng and Zeng, 2020). One solving scheme relies on competing self-focusing and defocusing terms, including cubic-guintic (Zeng and Malomed, 2012; Gao and Zeng, 2018) and cubic-guartic (Kartashov et al., 2018) nonlinearities. Quantum mechanical stabilization of a collapsing Bose-Bose mixture leads to quantum droplets (Petrov, 2015; Petrov and Astrakharchik, 2016; Cabrera et al., 2018; Semeghini., et al., 2018; Zhang et al., 2019), which, actually, derive from the competition of attractive mean-field term and repulsive beyond mean-field Lee-Huang-Yang correction (Lee et al., 1957) characterizing the quantum many-body effects (quantum fluctuations); in degenerate quantum gases, the nonlinearity is induced by atom-atom interactions and can be tuned by Feshbach resonance (Chin et al., 2010; Chen and Zeng, 2020; Kengne et al., 2021). Besides, linear periodic potentials are widely exploited for generating multidimensional optical and atomic matter waves (Ostrovskaya and Kivshar, 2003; Ostrovskaya and Kivshar, 2004; Alexander et al., 2005; Leblond et al., 2009; Zeng and Zeng, 2019; Li and Zeng, 2021; Chen and Zeng, 2021). Regular periodic structures, including photonic crystals and lattices in nonlinear optics and optical lattices in the context of ultracold atoms (Morsch and Oberthaler, 2006; Kartashov et al., 2011; Garanovich et al., 2012), offer new possibilities for studying one-dimensional gap solitons (Eiermann et al., 2004; Li and Zeng, 2021) and multidimensional gap solitons and vortices (Zeng and Zeng, 2019; Chen and Zeng, 2021) under the self-defocusing nonlinearity.

In 1998, Bender and collaborator found that the non-Hermitian systems conformed to the parity-time (PT) symmetry, counterintuitively, exhibit entirely real spectra (Bender and Boettcher, 1998). Intriguing characteristics of such systems (Bender, 2007) include exceptional point, PT symmetry breaking, and spectral singularities, whose physical relevance was confirmed in optical experiments in contexts of a lossy waveguide and coupled waveguides with gain and loss (Guo et al., 2009; Rüter et al., 2010). Recently there are growing research activities on PT-symmetric non-Hermitian systems with complex potentials whose



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real (imaginary) part is an even (odd) function in various fields of science and engineering (Konotop et al., 2016; Suchkov et al., 2016; Feng et al., 2017; El-Ganain et al., 2018; Miri and Alú, 2019). In particular, unconventional beam dynamics (Makris et al., 2008) and nonlinear waves (Musslimani et al., 2008; Kartashov et al., 2016) have been widely explored in \mathcal{PT} -symmetric systems (Konotop et al., 2016; Abdou et al., 2021; Zeng et al., 2021). The study of solitons in \mathcal{PT} -symmetric optical and photonic lattices is, however, limited to low-dimensional cases (Konotop et al., 2016; Suchkov et al., 2016; Zeng and Lan, 2012; Muniz et al., 2019; Zhu et al., 2013).

Theoretically, the PT symmetry can be manifested in Bose-Einstein condensates (BECs) by removing or loading atoms (for BECs placed in a double-well potential where atoms are injected in one well, whereas the atoms are removed from the second well) (Klaiman et al., 2008; Schwarz et al., 2017; Haag et al., 2018; Begun et al., 2021), and \mathcal{PT} -symmetric lattices can be realized in three-level Λ -type atomic gases using Raman resonances (Hang et al., 2013a, 2013b) and in multilevel atoms with more sophisticated atomic schemes (Hang et al., 2013a, 2013b; Wu et al., 2014; Wang and Wu, 2016). Subsequent experiments under the electromagnetically induced transparency (EIT) condition based on optical lattices technique have demonstrated the realizations of optically induced atomic lattices and the \mathcal{PT} symmetry therein (Zhang et al., 2018a, 2018b). It thus becomes possible to investigate the soliton physics in periodic \mathcal{PT} -symmetric lattices (Hang and Huang, 2017; Zhang et al., 2018a, 2018b). Recalling it remains an open question to explore the 3D nonlinear stabilization mechanism in \mathcal{PT} -symmetric potentials.

Using theoretical and numerical ways, we reveal the creation and stability issues of 3D localized matter-wave gap modes of two types—fundamental gap solitons and vortical ones with vorticity s = 1—in BECs loaded onto 3D \mathcal{PT} -symmetric optical lattices corresponding to different imaginary potential strengths; finding the stable matter-wave gap solitons and vortices occupy always the central part of the finite gaps in the associated linear band gap spectra. This work opens a new way for exploring and stabilizing 3D solitary gap states, providing in-depth understanding of soliton physics in multidimensional \mathcal{PT} periodic potentials beyond conventional Hermitian ones.

Theoretical model

Based on mean-field theory, the macroscopic matter-wave wave function (order parameter) U for dynamics of a BEC in 3D \mathcal{PT} -symmetric optical lattices is described in the framework of Gross-Pitaevskii equation, whose scaled form reads:

$$i\frac{\partial U}{\partial t} = -\frac{1}{2}\nabla^2 U + V_{PT}(\mathbf{r})U + g|U|^2 U, \qquad (\text{Equation 1})$$

here $\mathbf{r} = (x, y, z)$ and Lapalacian $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$, g > 0 (g < 0) represents the repulsive (attractive) atom-atom collisions (which, as aforementioned, can be managed by Feshbach resonance technique (Chin et al., 2010; Kengne et al., 2021)), and we set g = 1 throughout for discussion. The 3D simple \mathcal{PT} -symmetric periodic potential follows the expression:

$$V_{\mathcal{PT}}(x, y, z) = W_0 \{ \cos^2(x) + \cos^2(y) + \cos^2(z) + iV_0[\sin(2x) + \sin(2y) + \sin(2z)] \}$$
(Equation 2)

where W_0 is the modulation depth (amplitude) of the optical-lattice potential, and V_0 is the imaginary potential strength (gain-loss portion), whose periodicity is set to π . As a manifestation of non-Hermitian system, the configurable periodic potentials like that in Equation (2) indeed fulfill the necessary requirement of symmetry—the potential's real part is an even function, whereas its imaginary part is an odd, that is $V_{PT}(\mathbf{r}) = V_{PT}^*(-\mathbf{r})$. As stated earlier, the \mathcal{PT} -symmetric optical lattices with periodic varying gain and loss profiles may be induced in coherently prepared *m*-level systems (integer $m \ge 3$, atomic) (Hang et al., 2013a, 2013b; Wu et al., 2014; Wang and Wu, 2016; Zhang et al., 2016, 2018a, 2018b).

Stationary equation

The stationary localized-mode solution φ at defined chemical potential μ can be sought by $U = \varphi e^{-i\mu t}$; substituting it into the dynamical equation [Equation (1)] would result into the stationary equation:

$$\mu \varphi = -\frac{1}{2} \nabla^2 \varphi + V_{\mathcal{PT}}(\mathbf{r}) \varphi + \left| \varphi \right|^2 \varphi.$$
 (Equation 3)

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Figure 1. Linear band gap spectra for the 3D PT cubic lattice

(A–F) Matter-wave band gap spectra of a 3D PT cubic lattice corresponding to potential depth $W_0 \equiv 4$ and different imaginary potential strengths V_0 : (A) $V_0 = 0.05$; (B) $V_0 = 0.3$, and (C) $V_0 = 0.5$. Width of the first finite gap versus W_0 : (D) $V_0 = 0.05$ and (E) $V_0 = 0.3$. (F) The first Brillouin zone of the cubic lattice.

RESULTS AND DISCUSSION

Linear band-gap features

Considering that the 3D \mathcal{PT} -symmetric optical lattice (Equation 2) is a simple cubic lattice, for noninteracting condensate corresponds to the linearized Equation (3) (abandoning the last nonlinear term), the Bloch bands and forbidden gaps in the first reduced Brillouin zone presented in the reciprocal lattice space can be obtained by the linear Bloch theorem (which is widely used for deriving dispersion relation in crystalline solids and photonic crystals (Kivshar and Agrawal, 2003; Joannopoulos et al., 2008)). With this knowledge, the underlying matter-wave band gap properties of the considered 3D \mathcal{PT} optical lattice under three values of imaginary potential strength, $V_0 = 0.05$, $V_0 = 0.3$, and $V_0 = 0.5$, are displayed in Figures 1A-1C, respectively. There is a relatively wide first finite gap and a narrow second gap in the former two cases, whereas all the finite gaps close for the last case—a singularity property of \mathcal{PT} -symmetric periodic potentials at $V_0=0.5$, an effect of non-Hermitian degeneracy. Above such value, there is not any real eigenvalue (chemical potential μ) of the corresponding band-gap spectrum. It is of great interest and importance to see how the width of the first finite bandgap changes with an increase of potential depth; two typical examples of such relation at V₀=0.05 and V₀=0.3 are depicted respectively in Figures 1D and 1E, showing a linear growing relationship. Also for the sake of clarity, in Figure 1F, we show the corresponding first Brillouin zone in momentum (reciprocal) space expressed by the wave vectors, highlighting the high-symmetry points, R, X, and M.

Fundamental gap solitons

Because the formation and properties of band-gap structure of the 3D PT-symmetric optical lattice have been made clear, we can start looking into what the existence conditions of the corresponding nonlinear localized modes are and how to stabilize them. Characteristic profiles of 3D fundamental gap solitons under chemical potential $\mu = 4.1$ and $\mu = 4.8$ supported by the complex potential are depicted in the first and second columns of Figure 2; showings are also for the corresponding contour plots of the soliton's real part and the imaginary counterpart projected onto 2D plane at z = 0. It is clear that the real part of the gap soliton represents the highly localized mode, whereas its imaginary part is in a dipole shape—resembling their counterparts in physical settings



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Figure 2. Typical profiles of 3D fundamental gap solitons

Profiles of an unstable 3D fundamental gap soliton at chemical potential $\mu = 4.1$ (top, left) and a stable one at $\mu = 4.8$ (top, centre) supported by 3D \mathcal{PT} cubic lattice with potential depth $W_0 = 4$ and imaginary potential strength $V_0 = 0.05$. The top right panel displays an unstable gap soliton at $\mu = 8.5$ under $W_0 = 8$ and $V_0 = 0.05$. The central and the bottom lines are the corresponding real (U_r) and imaginary (U_i) parts of the solitons (expressed by wavefunction U) projected onto 2D plane at z = 0. The typical profiles of stable (top, centre) and unstable (top, left and right) gap solitons are corresponding to the marked points B, A, and C in Figure 3.

with low-dimensional \mathcal{PT} -symmetric periodic potentials (Zeng and Lan, 2012). As observed from the second column of Figure 2, going further deep inside the first gap (e.g., at $\mu = 4.8$), the side-peak modulation of the gap soliton increases, as the existence of a much stronger Bragg scattering, which, in principle, is induced by constructive interference of multiple coherently enhanced Bragg reflections in periodic potentials under the Bragg resonance condition (Kivshar and Agrawal, 2003; Joannopoulos et al., 2008). Displayed in the third column of Figure 2 is an unstable gap soliton at a larger lattice depth $W_0 = 8$; the soliton's amplitude increases accordingly. For the 3D \mathcal{PT} -symmetric optical lattice with small imaginary potential depth $V_0 = 0.05$, the relationship between atomic number N and chemical potential μ of the fundamental gap solitons within the first finite gap is collected in Figure 3A, where both the stability and instability regions are given, indicating stable cases in the midst of finite gap and unstable near the edges of gap, and particularly, N decreases sharply from the left edge of the gap to a minimum and then grows gradually. The soliton's amplitude (A_{max}) increases with an increase of μ ; the same decrease and growth tendency of N is for the radius of gap soliton (R_0)—the fundamental gap solitons may be approximated as 3D balls (as can be seen from Figure 2), according to Figure 3D. When closing to the upper edge of the first gap, the gap soliton expands itself (R_0 increases quickly) so as to fight against the strong Bragg scattering therein. For a moderate imaginary depth of the PT lattice, e.g., $V_0 = 0.3$, both the curves $N(\mu)$ and $A_{max}(\mu)$ develop in a different way compared with their counterparts at small V_0 ; such curves do not obey the simple linear increasing relationship again and the stability region narrows greatly, as observed from Figures 3B and 3E. By comparison, for gap solitons supported by a \mathcal{PT} cubic lattice

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Figure 3. Number of atoms, amplitude, and the corresponding radius versus chemical potential for 3D fundamental gap solitons Dependencies of number of atoms (*N*), amplitude (maximum value, A_{max}), and the corresponding radius R_0 on chemical potential μ for 3D fundamental gap solitons in the first finite gap. Potential depth $W_0 = 8$ for (C) and (F), $W_0 = 4$ for the rest; imaginary potential strength $V_0 = 0.3$ for (B) and (E), $V_0 = 0.05$ for the rest. The upper (red) and bottom (blue) curves in the right column panels depict the R_0 and A_{max} , respectively. The stability and instability regions of the gap solitons in all panels are depicted, respectively, by solid and dashed lines.

with a moderate potential depth $W_0 = 8$ as displayed in Figures 3C and 3F, there is a broader stability region, e.g., for $\mu \in [6.3, 8.3]$.

Gap vortices

Next, we find out how to excite gap vortices with imprinting topological charge (or vorticity) *s* and what stability properties they have. The gap vortices at *s* = 1 can be constructed as hollow quadruple structures composed of four bright peaks (fundamental gap solitons), which are entangled as a whole and spliced by $\pi/2$ phase shift between each peak. The relationship $N(\mu)$ for such gap vortices, supported by the 3D \mathcal{PT} -symmetric optical lattice with imaginary potential depth $V_0 = 0.05$, has been given through a large number of numerical studies (see the top panel of Figure 4), which is qualitatively akin to its counterpart for fundamental gap solitons in Figure 3A, and the difference is that the number of atoms is almost four times larger than that of a fundamental gap soliton. It should be noted that the stationary gap vortices very close to the left edge of the gap could not be constructed numerically; on account of their excited states property, this is very different from their fundamental ones. Typical examples of the gap vortices of two types, the parallelogram structure and square one, are illustrated respectively in the central and bottom lines of Figure 4; and the stability diagram of the first type gap vortices is more broader than that of the second type, which may be explained by the fact that the former keeps almost entirely the solitonic structure of the four individuals, whereas the latter is arranged in the most closest spacing, and the repulsive destructive effect between each gap soliton is nonnegligible.

Dynamics of 3D localized matter-wave gap modes

The perturbed evolutional dynamics of all the above-mentioned localized matter-wave gap modes, including the fundamental gap solitons and vortical ones, is displayed in Figure 5. In terms of an unstable fundamental mode, side peaks develop and spread during the time evolution, according to Figure 5A and the one supported by a larger potential depth in Figure 5C, whereas for the stable fundamental gap soliton

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Figure 4. Number of atoms versus chemical potential for 3D vortex gap solitons

Dependencies of number of atoms N on chemical potential μ for 3D vortex gap solitons with topological charge s = 1 (A) Curves $N(\mu)$ for 3D vortex gap solitons of on-site (red line) and off-site (blue line) types at $V_0 = 0.05$. Typical 3D profiles (left column), contour 2D densities |U| (central column) and the corresponding phases (right column) at z = 0 of on-site vortex gap soliton (central line) and off-site one (bottom line), marked by points C and D in upper panel. The solid and dashed lines in panel (a) correspond to the stable and unstable segments of solitons, respectively.

and gap vortex soliton, both the shape and coherence properties can be preserved well in the process of perturbed evolution (see Figures 5B and 5D); an unstable vortex soliton start to generate side peaks for an individual (single soliton) and such extra side peaks then affect the hollow quadruple structure and make it decay [Figure 5E]. In Figures 6A-6C, we depict the evolution of soliton's amplitude A_{max} for two unstable 3D fundamental gap solitons and an unstable vortex gap soliton at topological charge s = 1, revealing indepth amplitude details of the unstable evolutional cases displayed in Figures 5A, 5C, and 5E, respectively. It is observed that the unstable solitons oscillate slowly at the initial stage, and transform themselves into delocalized modes.

Conclusion

The non-Hermitian physics grounded on parity-time (PT) symmetry, originated firstly from the quantum mechanics, has attracted considerable theoretical and experimental attention in diverse branches of subjects, particularly in optics and photonics. PT-symmetrical potentials like periodic ones open a new possibility to generate and control nonlinear waves in non-Hermitian systems confined to low-dimensional spaces; exploring nonlinear wave localizations in full spatial dimension (3D) so far remains a missing topic. In this article, we have revealed, numerically and in an analysis, nonlinear self-trapping of matter waves in BECs with repulsive (defocusing) atom-atom interactions loaded into 3D PT-symmetric optical lattices,

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Figure 5. Dynamics of 3D fundamental gap solitons and vortices

(A–E) Perturbed evolutional dynamics of 3D fundamental gap solitons and gap vortices with topological charge s = 1. Perturbed evolution of the stable (B) and unstable (A, C) fundamental gap solitons and the stable (D) and unstable gap vortices (E). The initial states (at t = 0) in all panels correspond to the stationary solutions marked earlier added with random perturbation with strength equates 3% of the amplitude of solitons.

emphasizing the formation and dynamics of multidimensional matter-wave gap solitons and vortices. Noteworthy result is the finding of stable gap solitons and vortices with vorticity s = 1 supported by 3D \mathcal{PT} -symmetric optical lattices at small imaginary lattice depth [V_0 in Equation (2)], which can be realized in coherently multilevel atomic ensembles as demonstrated in recent experiments, and thus the predicted matter-wavelocalized gap modes are observable. Our study provides in-depth theoretical understandings of the formation, structural property, and dynamics of various coherent localized matter waves in non-Hermitian systems with multidimensional \mathcal{PT} optical lattices with periodical gain and loss profiles, offering a new avenue to the exploration and stabilization of 3D localized gap modes in non-Hermitian periodic systems.

Limitations of the study

Nonlinear wave localizations in 3D \mathcal{PT} -symmetric optical lattices have been revealed in this study, manifesting the fundamental gap solitons and vortices constructed within the first finite gap of the



Figure 6. Peak amplitude versus time for unstable 3D fundamental gap solitons and vortex one (A–C) Dependencies of peak amplitude A_{max} on evolution time t for two unstable 3D fundamental gap solitons (A, B) and an unstable vortex gap soliton with topological charge s = 1 (C), corresponding to the cases displayed in Figures 5A, 5C, and 5E respectively.





associated linear Bloch spectrum. To enrich our understanding of nonlinear localization mechanism in multidimensional periodic non-Hermitian systems, structuring the other structures of higher-order localized gap modes with and without topological charge (winding number) will be an interesting issue; another future study may pay attention to the formation and stability of 3D localized gap modes in two-mode model describing two-component BECs trapped by \mathcal{PT} -symmetric optical lattices.

STAR*METHODS

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AUTHOR CONTRIBUTIONS

J.W.L performed the numerical simulation and analysis; Y.P.Z jointly supervised this research; J.H.Z. conceived and guided this research and wrote the manuscript. All authors reviewed and edited the manuscript.

DECLARATION OF INTERESTS

The authors declare no competing interests.

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STAR*METHODS

KEY RESOURCES TABLE

REAGENT OR RESOURCE	SOURCE	IDENTIFIER
Software and algorithms		
Matlab (2017a)	Matlab Software Foundation	https://ww2.mathworks.cn
SMOM	(Yang, 2010)	https://epubs.siam.org/doi/pdf/10.1137/1.9780898719680.fm

RESOURCE AVAILABILITY

Lead contact

Further information and requests for resources and samples should be directed to and will be fulfilled by the lead contact, Jianhua Zeng (zengjh@opt.ac.cn).

Materials availability

This work did not generate new unique samples.

Data and code availability

All data reported in this paper will be shared by the lead contact upon request.

Code with instructions reported in this article will be shared by the lead contact upon request.

Any additional information required to reanalyze the data reported in this paper is available from the lead contact upon request.

METHOD DETAILS

Numerical methods

All the numerical results presented above are produced in this procedure: the stationary localized solutions are firstly constructed in the model Equation (3) using the modified squared-operator iteration method (MSOM) (Yang, 2010), then the stability properties of these solutions are evaluated in direct perturbed numerical simulations of the dynamical equation [see Equation (1)] by means of fourth-order Runge-Kutta method. In our simulations, the 3D spatial derivatives are integrated in fast Fourier transform recipe, and the computational spatial domain is confined to $(x, y, z) \in [-6\pi, 6\pi]$, with 256×256×256 spatial points, and the time step in direct perturbed simulations of Equation (1) is defined as $\Delta t = 0.001$.