ANALYTICAL DESCRIPTION OF THE NONLINEAR DYNAMICS OF BOSE-EINSTEIN CONDENSATES BY MEANS OF GENETIC ALGORITHMS

MIHAELA CARINA RAPORTARU[1], JANE JOVANOVSKI[2], BORO JAKIMOVSKI[2], DRAGAN JAKIMOVSKI[3], ANASTAS MISHEV[2]

[1]Horia Hulubei National Institute of Physics and Nuclear Engineering, Department of Computational Physics and Information Technologies, Reactorului 30, Magurele, Ilfov, Romania
E-mail: mraportaru@nipne.ro
[2]Ss. Cyril and Methodius University in Skopje, Faculty of Computer Science and Engineering, Rugjer Boshkovikj 16, Skopje, Macedonia
[3]Ss. Cyril and Methodius University in Skopje, Faculty of Natural Sciences and Mathematics, Arhimedova bb, Skopje, Macedonia

Received May 8, 2014

In this paper we show that parallel genetic algorithms provide an accurate analytical description of the nonlinear dynamics of a Bose-Einstein condensate. We consider a spherically symmetric condensate subject to periodic and aperiodic parametric excitations and show that the standard variational equation which describe the time-evolution of the condensate has simple analytical solutions. These solutions are obtained using parallel genetic algorithms and allow us to quantify analytically distinct physical processes such as resonant energy transfers and mode-lockings. The observed efficiency of this method for the aforementioned one-dimensional variational equation suggests that this method can be efficiently used for charting the stability spectrum of condensates subject to parametric excitations and possibly for the description of optic waves travelling in nonlinear media.

Key words: Nonlinear dynamics, Bose-Einstein condensates, analytic description, genetic algorithms.

1. INTRODUCTION

The experimental sturdiness of atomic Bose-Einstein condensates (BECs) [1] has turned them into the favourite testbed of nonlinear scientists of various backgrounds with substantial contributions coming from both experimental and theoretical research groups [2]. Part of the interest in working with these ultra-cold quantum gases came from their experimental manoeuvrability (which generated a surge of investigations which go from nonlinear pattern formation and parametric excitations of collective modes to solitons and vortices) and their accurate dynamical description in a vicinity of $T = 0$ K using a cubic nonlinear Schrödinger equation, the so-called Gross-Pitaevskii equation (GPE) [3, 4]. The numerous similarities between the GPE and the equation used in optics to describe quasi-monochromatic wave trains propagating in nonlinear optical media (see Ref. [5] for a review on the nonlinear waveforms supported by this equation), as well as the similarities with the equations used

to model superconductivity, the water-wave problem, the Langmuir oscillations and the Alfvén waves that arise in plasma physics (see Ref. [6] for a detailed presentation), motived many of the early theoretical investigations into the nonlinear phenomena. In fact, the study of BECs has attracted scientists from fields as diverse as nonlinear mechanics and statistical physics, quantum optics and nuclear physics and condensed matter physics and nonlinear optics, and as recognition of this almost unprecedented scientific effervescence the experimentalists who first achieved the Bose-Einstein condensation of atomic species in 1995 received the 2001 Nobel Prize in Physics.

In this paper we investigate the dynamics of a spherically symmetric BEC subject to periodic and aperiodic parametric excitations through parallel genetic algorithms. Unlike previous studies, we combine the habitual variational treatment of BECs with a High Performance Computing (HPC) genetic algorithm to describe analytically the dynamics of the condensate during parametric resonances [7], resonant energy transfers [8] and mode-lockings [9]. The strong points of the genetic algorithm are that it can be applied independent of the density regime of the condensate and that it is intrinsically parallel and thereby computationally efficient on large computer clusters. We emphasize that unlike other approaches which aim at reducing the computational time by rethinking the initial quantum many-body problem itself, see, for example the ultra-fast path-integral methods for the dynamics of quantum gases detailed in [10] and the related ones for quantum gases in optical lattices [11], our method addresses the actual equations which describe the dynamics of the condensates without going outside of the Gross-Pitaevskii formalism. Outside of quantum gases, we expect that genetic algorithms can be used in nonlinear optics to reduce the computational load in the laser physics investigations such as those focused on gain and ionization dynamics [12], chirped pulse amplification [13], the focal region of ultrashort laser pulses [14], and compensation of laser beam spatial distortions [15].

The rest of the paper is structured as follows: in Section 2 we introduce the variational treatment of BECs, while in Section 3 we present the fundamentals of the genetic algorithm used to solve the variational equation. Section 4 is dedicated to presenting our results and in Section 5 we present our concluding remarks.

2. VARIATIONAL DESCRIPTION OF BOSE-EINSTEIN CONDENSATES

The numerical treatment of the GPE is well-covered in the literature and there exist two classical sets of programs in Fortran [16] and C++ [17] which describe the time evolution of one-, two- and three-dimensional BECs subject to time modulation of the confining potentials and that of the scattering length. Outside the purely numeric treatment the dynamics of quasi-one-dimensional and quasi-two-dimensional BECs can be described through simplified non-polynomial equations (see Refs. [18–

20] for low-density condensates and Refs. [21–23] for high-density ones) and there are similar extensions for binary condensates. The equations for low-density condensates have been particularly useful in the early investigations into the nonlinear dynamics of BECs due to their reduced computational burden (see Ref. [20] and references therein), but the recent OpenMP parallelized version of the numerical GPE solvers make them more interesting for analytical investigations. Complementary analytical investigations have been focused on a hydrodynamic [24] and fully-variational description [25–37] of BECs using trial wave functions which could describe the collective properties of the condensates and the emergence of density waves. Unlike the non-polynomial Schrödinger equations, the variational recipes previously mentioned simplified the dynamics of the condensate to the level of a few ordinary differential equations which can be easily solved numerically through classical methods such as Runge-Kutta and Adams-Bashforth [38]. Specific properties condensates (such as the frequency of the collective modes and the period of the density waves) can be obtained solely by analytical means, but for all other information concerning the dynamics of condensate one has to solve numerically the variational equations.

For the purpose of this paper we will focus on a condensate with spherical symmetry subject to periodic and aperiodic modulation of the scattering length following the treatment in Refs. [9, 8]. To describe analytically the dynamics of the condensate we consider the standard three-dimensional GP Lagrangian density [1] (written here for convenience with $m = \hbar = 1$ all throughout the article)

$$\mathcal{L}(\mathbf{r},t) = \frac{i}{2}\left(\psi\frac{\partial\psi^*}{\partial t} - \psi^*\frac{\partial\psi}{\partial t}\right) + \frac{1}{2}\left|\nabla\psi\right|^2 + V(\mathbf{r},t)\left|\psi\right|^2 + \frac{g(t)N}{2}\left|\psi\right|^4 \tag{1}$$

loaded in a trap of the form

$$V(\mathbf{r},t) = \frac{1}{2}\Omega^2 r^2. \tag{2}$$

Given the symmetry of the system the most convenient ansatz is

$$\psi(r,t) = A(t)\exp\left[-\frac{r^2}{2w(t)^2} + ir^2\beta(t)\right], \tag{3}$$

where $A(t)$ is the complex-valued wave-function at the centre of the cloud, $w(t)$ is the width of the condensate and $\beta(t)$ is the canonical conjugate of $w(t)$. Following the standard variational recipe we arrive at a second-order ordinary differential equation

$$\frac{d^2}{dt^2}w + \Omega^2 w = \frac{1}{w^3} + \frac{g(t)}{2\sqrt{2}}\frac{N}{\pi^{3/2}w^4} \tag{4}$$

which is usually written as

$$\frac{d^2}{d\tau^2}v + v = \frac{1}{v^3} + \frac{P(t)}{v^4}, \tag{5}$$

where $v = w\sqrt{\Omega}$ and $\tau = \Omega t$.

3. GENETIC ALGORITHMS

A system of ordinary (SODE) or partial differential equations is so an ubiquitous model in applied science that is so naturally met with equally diverse methods for its solution, ranging from standard Runge-Kutta [39] to more exotic use of neural networks [40]. The genetic algorithms (GA), are a class of optimization processes based on the evolution of a large number of candidate solutions, specific for the problem in hand, through evolutionary inspired operations of crossover, mutation and replication and ultimately of surviving of the best solution [41]. These strategies for solving various scientific and engineering problems are usually more robust and reliable in optimization tasks when the complexity of the solution is unknown beforehand and one expects that it is highly non-trivial.

In context of physics, evolutionary methods were successfully applied to a representative selection of problems, from solving of general eigenvalue problem with GA [42], via direct solving of the Schrödinger equation [43, 44], to more complex systems with two electrons [45] or hydrogenic impurity in a quantum dot [46]. Various combinations with other computational techniques were also widely addressed. To this end the community developed a few rather sophisticated software packages.

In this work we have used the free PGAPack Parallel Genetic Algorithms Library, release 1.0, developed mainly by David Levine from Argonne National Library [47]. This software package offers the user wide range of choices of the parameter values, operators and algorithms for the selection, crossover and mutation phases of each GA implementation, in an integrated and portable way and it may be called from Fortran and executed on platforms with one or several processors.

The user of PGAPack supply a function with several parameters to be optimized under fixed conditions. As initial guess we have used functions with several real parameters. With each run these parameters have been initialized to a population of strings, with values from a fixed interval, specific for each parameter, and allow for the program to extend the range of possible values on parameter values fly, if needed, during the optimization process. From the available mutation and crossover types we opted for uniform varieties in both cases as this choice is neutral in respect of searching flexibility.

As a measure, relative to the rest of population of parameters, how well each set of parameters is fit we used a cost-function, rule to assign to each string a non-

negative, real-valued fitness. This problem-specific metric consists of two parts. The first, boundary part, includes the squared distances of the candidate solution, from the initial values and from boundary points, if there are any, as well as from a set of fixed points of the solution to be found, itself. In our problem we have expressed our differential equation as a system of two first order equations, with respective initial conditions and explicitly found the derivatives from the general form ansatz. The second part of the cost-function then consists of the squared distances between the values of the candidate solution and the analytical solution from the system of differential equations at a fixed number of points, in our case 2000 which span the time interval. These two-parts of the cost-function, equation part and boundary part compete in optimization process with different weights, in our calculations 1:300, which means the boundary part has 300 times more "to say" if the candidate solution is fit enough or not, compared to equation part. As an additional restrain we included an ad-hoc penalty in the fitness part if the candidate solution generates function values outside some fixed range where we expect that there should not be any.

In case of an ideal solution, the cost-function, constructed in this way, should be equal to zero. It means that at each of the 2000 points, the candidate analytical solution with an optimized set of parameters, satisfies perfectly our equation (correct functions and their derivatives) as well as the initial conditions and matches the set of fixed points, with no penalty whatsoever. In practice this convergence toward analytical solution is compromised at several levels. First, the proposed analytical ansatz may not be a solution of the equation at hand and the equation itself may not have such solution at all. This weakness may be addressed with more general form of a function with larger set of parameters to choose from but this "solution" may be time-consuming without proof that the proposed function is good enough. On the other hand, the convergence may be slow due to large number of local minima in the optimization space where the program gets stuck. One of the remedy for this problem, larger mutation rate, may be prohibitively time-consuming too.

So, as a first step toward our solution we have expressed equation (5) as a system

$$\frac{dv_1}{dt} + v - \frac{1}{v^3} - \frac{P[1+\varepsilon\sin(\gamma t^2)]}{v^4} = 0\,; \quad \frac{dv}{dt} = v_1 \tag{6}$$

to be solved in interval $t \in [a, b]$, in our numerical experiments set to $[0, 200]$.

We have run numerical experiments with several sets of ansatz functions of the form:

$$y(x) = \sum_i^n \frac{\left(a_i + b_i sin(c_i x + d_i) + e_i sin(g_i x^2 + h_i)\right)}{1 + e^{(j_i(k_i - x))}} \tag{7}$$

where $a_i, b_i, \ldots$ are parameters to be optimized; n was in a range of 1 to 5, $9n$ being

the total number of parameters. And,

$$y(x) = \left[ax + \sqrt{((x^b \sin(cx+d))^2 + e)}\right] \left[\sqrt{\left((\sin^2(fx+g)+h)\right)}\right] \tag{8}$$

where $a, b, c \ldots$ are parameters to be optimized. The form of a chromosome in population is a vector of respectively $9n$ or 8 real numbers.

The ansatz functions are analytic and their first derivative $yp(x)$ and higher ones, can easily be found and they have been implemented in the code when cost function has been calculated. The cost function itself, in our runs, consists of three parts: C_1 to C_3, represented by

$$C_1 = \sum_i^N (y(t_i) - yp(t_i))^2 + ((yp(t_i) + y(t_i)) * y(t_i)^4 - y(t_i) - P[1 + \varepsilon \sin(\gamma t_i^2)])^2 \tag{9}$$

where t_i are the first points of the N equidistant subintervals of $[0, 200]$.

$$C_2 = yp(t_1)^2 + (y(t_1) - 2.52444)^2 + \sum_k^n (y(t_k) - y_{ex}(t_k))^2 \tag{10}$$

where t_k are n selected time moments for which the exact values y_{ex} of the solution are supposed to be known; in our numerical experiments we choose $n = 10$ from a total of $N = 2000$ points. And, the third part of the cost function was a penalty, large arbitrary constant, $C_3 = 10^9$ which was added ad-hoc if the candidate solution happens to be larger or smaller then supposed values of the solution. This last part effectively "squeezes" the values of the candidate solution within some vertical span of possible values. The final form of the cost function combines C_2 part with a weight, as explained previously, as $C = C_1 + w_2 C_2 + C_3$, w_2 being in general in range 300 to $3 * 10^5$.

4. RESULTS

To test the efficiency of the genetic algorithms detailed above for the solution of the ordinary differential equations which describe the nonlinear dynamics of BECs, we have chosen a challenging scenario in which the two-body scattering length is modulated as $P(t) = P_0 \cdot (1 + \epsilon \sin(\gamma t^2))$. Such a modulation is well known to give rise to both frequency mode-locking and resonant energy transfer (see Ref. [9] and Ref. [8]) and is therefore the ideal test case.

The results presented in Figure 1 show that genetic algorithms have provided a solution which captures the full physics of the problem, albeit with some quantitative discrepancies. Notice that the condensate has an almost negligible dynamics until

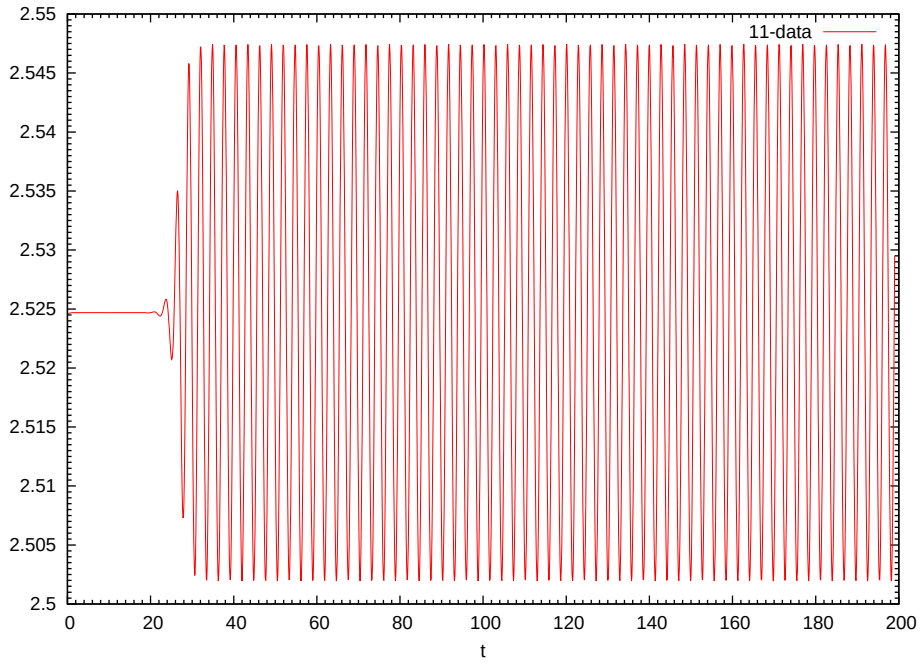

Fig. 1 – The dynamics of the width of the condensate for $P = 100$, $\epsilon = 0.01$ and $\gamma = 0.05$. Time is measured in milliseconds. The condensate starts to oscillate periodically at roughly 25 milliseconds which is precisely when the effective frequency of the drive matches the natural frequency of the condensate. This example corresponds to 24.500 atoms of ^{23}Na loaded into a magnetic trap with a frequency of 159 Hz and has been initially addressed in Ref. [9].

the effective frequency of the drive $2\gamma t$ matches the natural frequency of the system and that just when the two have almost equal value we observe a sudden increase of the oscillation amplitude due to resonant energy transfer, while for larger effective driving frequencies the condensates shows oscillations at the natural frequency of the system. These two effects are linear in nature and have been explained in detail in Ref. [8] using Fresnel functions. The advantage of our description is that it offers almost the same quantitative results using, however, substantially simpler functions which are amenable to subsequent analytic manipulations.

5. CONCLUSIONS

In this paper we have shown that parallel genetic algorithms provide an accurate analytical description for the frequency mode-locking and resonant energy transfer that take place in a spherically symmetric Bose-Einstein condensate subject to parametric excitations. The quasi-analytic solutions we have determined so far suggest that parallel genetic algorithms are powerful computational instruments

which allow one to quantify analytically numerous physical processes in ultra-cold quantum gases.

Acknowledgements. The authors thank A.I. Nicolin and M. Dulea for numerous fruitful discussions. The work of M.C. Raportaru is funded by Romanian Ministry of Education through project PN 09370104/2014. The authors acknowledge the use of resources provided by the NGI MARGI, as part of the European Grid Infrastructure.

REFERENCES

1. C.J. Pethick and H. Smith, *Bose-Einstein Condensation in Dilute Gases* (Cambridge University Press, Cambridge, 2008).
2. P.G. Kevrekidis, D.J. Frantzeskakis, and R. Carretero-González (Eds.), *Emergent Nonlinear Phenomena in Bose-Einstein Condensates* (Springer, Berlin, 2008).
3. E.P. Gross, Nuovo Cim., **20**, 454 (1961).
4. L.P. Pitaevskii, Zh. Eksp. Teor. Fiz., **40**, 646 (1961).
5. B.A. Malomed, D. Mihalache, F. Wise, and L. Torner, J. Opt. B: Quantum Semiclass. Opt., **7**, R53 (2005).
6. C. Sulem and P.-L. Sulem, *The nonlinear Schrödinger equation* (Springer, New York, 1999).
7. I. Vidanović, A. Balaž, H. Al-Jibbouri, and A. Pelster, Phys. Rev. A **84**, 013618 (2011);
   H. Al-Jibbouri, I. Vidanović, A. Balaž, and A. Pelster, J. Phys. B: At. Mol. Opt. Phys. **46**, 065303 (2013);
   W. Cairncross and A. Pelster, Eur. Phys. J. D **68**, 106 (2014).
8. A.I. Nicolin, M.H. Jensen, J.W. Thomsen, and R. Carretero-González, Physica D, **237**, 2476 (2008).
9. A.I. Nicolin, M.H. Jensen, and R. Carretero-González, Phys. Rev. E, **75**, 036208 (2007).
10. A. Balaz, A. Bogojevic, I. Vidanovic, and A. Pelster, Phys. Rev. E **79**, 036701 (2009);
    A. Balaz, I. Vidanovic, A. Bogojevic, A. Belic, and A. Pelster, J. Stat. Mech. P03004 (2011);
    A. Balaz, I. Vidanovic, A. Bogojevic, A. Belic, and A. Pelster, J. Stat. Mech. P03005 (2011).
11. G.J. Dong, J. Zhu, W.P. Zhang, and B.A. Malomed, Phys. Rev. Lett. **110**, 250401 (2013);
    M. Mobarak and A. Pelster, Laser Phys. Lett. **10**, 115501 (2013);
    T. Wang, X.-F. Zhang, S. Eggert, and A. Pelster, Phys. Rev. A **87**, 063615 (2014).
12. D. Ursescu and L. Ionel, J. Opt. Adv. Mat. **12**, 48 (2010).
13. L. Ionel, Opt. Adv. Mat. - Rapid Comm. **7**, 481 (2013).
14. L. Ionel and D. Ursescu, Rom. Rep. Phys. **62**, 500 (2010).
15. L. Ionel, Rom. Rep. Phys. **65**, 984 (2013).
16. P. Muruganandam and S.K. Adhikari, Comp. Phys. Comm., **180**, 1888 (2009).
17. D. Vudragovic, I. Vidanovic, A. Balaz, P. Muruganandam, and S.K. Adhikari, Comp. Phys. Comm., **183**, 2021 (2012).
18. L. Salasnich, A. Parola, and L. Reatto, Phys. Rev. A **65**, 043614 (2002).
19. L. Salasnich, Laser Phys. **12**, 198 (2002).
20. L. Salasnich, J. Phys. A: Math. Theor. **42**, 335205 (2009).
21. A.I. Nicolin, Rom. Rep. Phys. **61**, 641 (2009).

22. A.I. Nicolin and M.C. Raportaru, Physica A **389**, 4663 (2010).
23. A. Muñoz Mateo, V. Delgado, Phys. Rev. A **77**, 013607 (2008).
24. F. Dalfovo, C. Minniti, and S. Stringari, Phys. Lett. A **227**, 259 (1996).
25. V.M. Pérez-García, H. Michinel, J.I. Cirac, M. Lewenstein, and P. Zoller, Phys. Rev. Lett. **77**, 5320 (1996).
26. V.M. Pérez-García, H. Michinel, J.I. Cirac, M. Lewenstein, and P. Zoller, Phys. Rev. A **56**, 1424 (1997).
27. A.L. Fetter, J. Low. Temp. Phys. **106**, 643 (1997).
28. K.S. Fa, R.S. Mendes, P.R.B. Pedreira, and E.K. Lenzi, Physica A **295**, 242 (2001).
29. E. Erdemir and B. Tanatar, Physica A **322**, 449 (2003).
30. A.I. Nicolin and R. Carretero-Gonzáles, Physica A **387**, 6032 (2008).
31. A.I. Nicolin and M.C. Raportaru, Proc. Rom. Acad. **12**, 209 (2011).
32. A.I. Nicolin, Phys. Rev. E **84**, 056202 (2011).
33. A.I. Nicolin, Physica A **391**, 1062 (2012).
34. M.C. Raportaru, Rom. Rep. Phys. **64**, 105 (2012).
35. A. Balaz and A.I. Nicolin, Phys. Rev. A **85**, 023613 (2012).
36. A.I. Nicolin, Proc. Rom. Acad. **14**, 35 (2013).
37. S. Balasubramanian, R. Ramaswamy, and A.I. Nicolin, Rom. Rep. Phys. **65**, 820 (2013); A. Balaz, R. Paun, A. I. Nicolin, S. Balasubramanian, and R. Ramaswamy, Phys. Rev. A **89**, 023609 (2014).
38. L.F. Shampine, *Numerical Solution of Ordinary Differential Equations* (Chapman&Hall, New York, 1994).
39. J.D. Lambert, *Numerical methods for ordinary differential systems: the initial value problem* (John Wiley&Sons, Inc. 1991).
40. I.E. Lagaris, A. Likas, and D.I. Fotiadis, IEEE Trans. Neural Networks, **9**, 987 (1998).
41. D.E. Goldberg, *Genetic Algorithms in Search, Optimization and Machine Learning* (Addison-Wesley Longman Publishing Co., Inc. 1989).
42. S. Nandy, R. Sharma, S.P. Bhattacharyya, *Solving symmetric eigenvalue problem via genetic algorithms: Serial versus parallel implementation*, Appl. Soft Computing, **11**, 3946 (2011).
43. P. Chaudhury, S.P. Bhattacharyya, *Numerical solutions of the Schrödinger equation directly or perturbatively by a genetic algorithm: test cases*, Chem. Phys. Lett. **296**, 51 (1998).
44. R. Saha and S.P. Bhattaccharyya, *On directly solving radial Schrödinger equation for the ground states of two electron atoms or ions by genetic algorithm*, J. Theor. Comp. Chemistry, **3**(3), 325 (2004).
45. I. Grigorenko and M.E. Garcia, *Ground-state wave functions of two-particle systems determined using quantum genetic algorithms*, Physica A **291**, 439 (2001).
46. M. Sahin, Ü Atav and M. Tomak, *Applications of Genetic Algorithm to Quantum Mechanical Systems*, Turk. J. Phys. **30**, 253 (2006).
47. D. Levine *PGApack* Mathematics and Computer Science Division, Argonne National Laboratory, 1995
48. C. Ridders, Advances in Engineering Software, **4**, 75 (1978).