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Numerical modeling of exciton–polariton Bose–Einstein condensate in a microcavity☆

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ABSTRACT

A novel, optimized numerical method of modeling of an exciton–polariton superfluid in a semiconductor microcavity was proposed. Exciton–polaritons are spin-carrying quasiparticles formed from photons strongly coupled to excitons. They possess unique properties, interesting from the point of view of fundamental research as well as numerous potential applications. However, their numerical modeling is challenging due to the structure of nonlinear differential equations describing their evolution. In this paper, we propose to solve the equations with a modified Runge–Kutta method of 4th order, further optimized for efficient computations. The algorithms were implemented in form of C++ programs fitted for parallel environments and utilizing vector instructions. The programs form the EPCGP suite which has been used for theoretical investigation of exciton–polaritons.

Program summary

Program title: EPCGP

Catalogue identifier: AFBQ_v1_0

Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AFBQ_v1_0.html

Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland

Licensing provisions: BSD-3

No. of lines in distributed program, including test data, etc.: 2157

No. of bytes in distributed program, including test data, etc.: 498994

Distribution format: tar.gz

Programming language: C++ with OpenMP extensions (main numerical program), Python (helper scripts).

Computer: Modern PC (tested on AMD and Intel processors), HP BL2x220.

Operating system: Unix/Linux and Windows.

Has the code been vectorized or parallelized?: Yes (OpenMP)

RAM: 200 MB for single run

Classification: 7, 7.7.

Nature of problem: An exciton–polariton superfluid is a novel, interesting physical system allowing investigation of high temperature Bose–Einstein condensation of exciton–polaritons-quasiparticles carrying spin. They have brought a lot of attention due to their unique properties and potential applications in polariton-based optoelectronic integrated circuits. This is an out-of-equilibrium quantum system confined within a semiconductor microcavity. It is described by a set of nonlinear differential equations similar in spirit to the Gross–Pitaevskii (GP) equation, but their unique properties do not allow

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standard GP solving frameworks to be utilized. Finding an accurate and efficient numerical algorithm as well as development of optimized numerical software is necessary for effective theoretical investigation of exciton–polaritons.

Solution method: A Runge–Kutta method of 4th order was employed to solve the set of differential equations describing exciton–polariton superfluids. The method was fitted for the exciton–polariton equations and further optimized. The C++ programs utilize OpenMP extensions and vector operations in order to fully utilize the computer hardware.

Running time: 6h for 100 ps evolution, depending on the values of parameters

1. Introduction

In this paper we propose a novel, optimized numerical method of modeling exciton–polariton superfluid in a semiconductor microcavity. Excitons are electron–hole pairs, bound by the Coulomb force, behaving as a single electrically-neutral particle [1,2]. Microcavities pumped by laser beams confine light in the form of a standing wave between highly reflective Bragg mirrors, which are made from multiple layers of different refractive index, see Fig. 1. Between the reflectors there are located semiconductor quantum wells where the excitons are formed and can freely move in the X–Y plane. If the wells are located in the anti-nodes of the standing wave, they strongly couple to photons and thus, they form new quasiparticles—the exciton–polaritons.

Strong coupling between photons and excitons is revealed with their dispersion relation. Photons in the microcavity possess quadratic dispersion relation. The dispersion of bulk excitons is approximately constant due to their relatively large mass. In the weak coupling regime, the two curves cross. However, solving the Schrödinger equation for the strongly coupled system yields two anti-crossing eigenstates called upper (UP) and lower exciton–polaritons (LP), Fig. 2. The energy difference between LP and UP is called the Rabi splitting. An excellent review on exciton–polaritons can be found in [3,4].

Exciton–polaritons are an out-of-equilibrium quantum system due to the interplay between their lifetime, up to 200 ps, and laser pumping sustaining their number in the cavity. The compound nature of polaritons results in the fact that their effective mass is lower than the mass of a free electron, and in the regime of their low density they can be described as bosons with a spin degree of freedom [5,6,3]. Thus, in specific conditions, they form a quasi-particle counterpart of an atomic Bose–Einstein condensate (BEC) [4,7] and reveal superfluidity [8] in relatively high temperatures [9].

Except for their amazing physical properties being a subject of the fundamental research, recently exciton–polaritons have brought a lot of attention due to their potential applications in optoelectronic integrated circuits, consisting of transistors [10], spin-switches [11] and logic gates [12–14]. Additionally, they can form localized nondiffracting X-waves [15,16] which could be used for transferring a classical signal between elements in the circuits. Thus, polaritonics is regarded as a future of new photonic–electronic devices, which will be capable of processing information at a rate of terabits per second and frequencies in the range 100 GHz–10 THz [17].

The simplest physical model of the exciton–polariton superfluid is given by the Gross–Pitaevskii equation (GPE). This is a nonlinear Schrödinger equation, which omits the quasi-particle nature of polaritons and which was primarily used for studying an akin discipline—the physics of ultracold quantum bosonic gases (of atoms) and their BECs. For this reason, over the years, a variety of numerical methods of solving GPEs were developed and implemented in software. They range from the most general, suitable for broad investigation of the gases, to specially fitted to specific systems and problems. Most papers devoted to numerical investigation of GPEs focused on their stationary solutions [18]. Various condensate geometries [19], simplifications and special cases [20] were taken into account. Numerical methods involved finite-difference approach [19,21,22], bi-k-Lagrange elements [23], spectral collocation methods with Chebyshev polynomials of the first and second kind [24] as well as basis set expansion technique [25]. Time-dependent equations were solved with implicit and semi-implicit Crank–Nicolson methods [18,26–29], Euler scheme [22], third and fourth-order adaptive Runge–Kutta methods [30], split-step finite difference method [22] and time-splitting sine and Fourier pseudospectral methods [31,32]. In the latter case, space was discretized with second- and fourth-order finite differences, exponential splines [29] or with Chebyshev–Tau spectral discretization method [26].

As a result, several mature software packages were developed. The OCTBEC utilizes optimal quantum control theory to model various BECs in Matlab [33]. Similar libraries were prepared in Fortran [18] and C programming languages [32]. The most advanced toolkit is the GPELab, implemented in Matlab [34,35]. It combines various listed methods in order to solve both stationary and time-dependent GPEs and enables tackling sets of equations. The hardware utilized for computations involved diverse platforms: OpenMP and MPI-based computer clusters [36], NVIDIA's CUDA parallel architecture [37,38] as well as Sony PlayStation 3 Cell Broadband parallel systems [39].

Deeper insight into the physics of polaritons requires however taking into account their compound character and solving a GPE for a spinor polariton wave function, consisting of two independent components: the excitonic ψ_x and photonic ψ_c one. This turns the GPE into a system of two coupled equations of different kind, of which neither is a GPE itself and thus, methods developed for solving GPEs cannot be directly applied. Further including of the spin degree of freedom for polaritons results in the system of four equations.

Here we present the EPCGP program suite which we have developed in order to support research on exciton–polaritons in semiconductor microcavities. The suite utilizes our novel algorithm based on the Runge–Kutta method of fourth order, optimized for the equations describing exciton–polariton superfluid. Moreover, program routines are able to gain from the parallel computing environment and vector operations, which significantly speeds up the computations. It allows investigation of one- and two-dimensional systems. We believe that use of EPCGP suite goes beyond the basic theoretical work and will also find applications in preparation of experiments and engineering of polaritonic circuits.

The paper is structured as follows. Section 2 introduces the Reader to the equations describing the exciton–polariton superfluid. Section 3 goes into details of numerical computations, presenting the choice of algorithms, data structures and properties of the methods, such as their stability, computational complexity and error estimation. Next, Section 4 presents a selection of interesting results obtained