Simulation of equilibrium particle distribution of the Bose gas of polaritons using quantum Monte Carlo

I O Kuznetsov and P F Kartsev
National Research Nuclear University “MEPhI” (Moscow Engineering Physics Institute), Kashirskoe sh. 31, 115409 Moscow, Russia
E-mail: PFKartsev@mephi.ru

Abstract. We present a numerical approach to study the system of exciton polaritons in an optical resonator under pumping. First task in this problem, is to determine the stationary particle distribution. In the case of low enough temperature, to describe the system correctly one cannot neglect the correlations between particles (including the Bose-Einstein condensate) and should take into account all interaction types present in the model. One of the most promising approaches to describe many-particle interacting systems, is the Quantum Monte Carlo (QMC) method. In this article, we describe a modification of the trajectory algorithm based on the Continuous Time World-Line (CTWL) QMC method to simulate the polaritonic system for various parameters of the problem. The modification is described in details.

1. Introduction
The weakly-interacting Bose gas has generated new wave of interest last years, due to new experimental problem of the excitonic polaritons in semiconductor under laser pumping in optical cavity [1, 2]. The interest is explained by the possibility of reaching the state of Bose-Einstein condensation (BEC) at high enough temperature.

The state of BEC is the result of the thermal equilibrium distribution of particles. To reach the equilibrium state, the interparticle interaction should be strong enough. The rate of relaxation and BEC formation must be faster than harmful processes such as exit of photons and decay of excitons [3].

The polaritonic system is a subject for large count of theoretical [2, 4] and experimental [5] studies. Among others, appearance of superfluidity [6] and quantized vortices [7] can be named. The spontaneous transitions in the polaritonic system, including laser applications, are studied in [7, 8]. The so-called “polaritonic laser” is discussed when the coherent generation due to spontaneous recombination of polaritons leads to the condensate deterioration [9, 10]. A significant number of theoretical [11, 12] and experimental works is dedicated to the BEC dynamics in this system [13].

Considering the interest to the system, reliable theoretical model should be useful to determine the optimal parameters of the experiment. Complex model of interactions leads to the need of taking into account the perturbation terms of high orders. The method of Quantum Monte Carlo [11, 12, 14] is one of the promising numerical approaches to interacting quantum systems.

In this report, we describe the modification of the Worm algorithm [15] based on the diagrammatic QMC method [16] designed for the polaritonic system.
2. Model
The system under study consists of two subsystems — excitons and photons — connected with Rabi coupling $\Omega$. Photonic subsystem is coupled to the external electromagnetic field $\mathbf{G}_k$ reflecting optical pumping and finite lifetime of photons in the resonator. Excitonic subsystem includes interparticle interaction $U_0$ and amplitude of particle decay $R_k$. The Hamiltonian of the composite system is written as:

$$H_{pol} = \sum_k \left( E^{(cav)}_k - \mu \right) \hat{a}_k^+ \hat{a}_k + \sum_k \left( E^{(exc)}_k - \mu \right) \hat{b}_k^+ \hat{b}_k + \hbar \Omega \sum_k \left( \hat{a}_k^+ \hat{b}_k + \hat{a}_k \hat{b}_k^+ \right) +$$

$$+ U_0 \sum_{klp} \hat{b}_l^+ \hat{b}_p \hat{b}_{k+l-p} + \sum_k \left( \mathbf{G}_k \hat{a}_k^+ + \mathbf{G}_k^* \hat{a}_k \right) + \sum_k \left( R_k \hat{b}_k^+ + R_k^* \hat{b}_k \right),$$

where the operators of photonic and excitonic parts are denoted by $\hat{a}^+, \hat{a}$ and $\hat{b}^+, \hat{b}$, respectively, and $E^{(cav)}_k$, $E^{(exc)}_k$ are the dispersion laws for the cavity photon and exciton, respectively. The chemical potential $\mu$ is introduced to control the total number of particles.

3. Quantum Monte Carlo
In diagrammatic QMC, each perturbation diagram is represented by the configuration of particle trajectories (worldlines) in the imaginary time $\tau = 0 \ldots \beta$, where $\beta \equiv 1/k_B T$. Each term of the Hamiltonian gives either the corresponding worldline change (the so-called kink), for example hopping between sites, or the propagation of the worldline along the imaginary time axis. During the simulation, the Monte Carlo configurations are transformed into each other using stochastic changes of the worldlines (updates), with their correct statistical weight guaranteed by the Metropolis algorithm.

The numerical simulation of such system with fixed temperature will give the established distribution of Bose particles under condition of constant external pumping and outflow from the system. Here we neglect the interaction between excitons and lattice phonons which can result in cooling of the polaritons, but with characteristic time much longer compared to the times of other processes in the system. This term, nevertheless, can be introduced into model as the third subsystem — phonons. New terms in the Hamiltonian (1) would then enter the QMC simulation with the appropriate types of kinks and updates.

In order to simplify the simulation process, we transform the Hamiltonian (1) to real space:

$$H_{pol} = -\mu \sum_i \left( \hat{a}_i^+ \hat{a}_i + \hat{b}_i^+ \hat{b}_i \right) - t^{(cav)} \sum_{i<j>} \hat{a}_i^+ \hat{a}_j - t^{(exc)} \sum_{i<j>} \hat{b}_i^+ \hat{b}_j + \hbar \Omega \sum_i \left( \hat{a}_i^+ \hat{b}_i + \hat{a}_i \hat{b}_i^+ \right) +$$

$$+ \sum_i \left( \mathbf{G}_i \hat{a}_i^+ + \mathbf{G}_i^* \hat{a}_i \right) + \sum_i \left( R_i \hat{b}_i^+ + R_i^* \hat{b}_i \right),$$

where the coefficients in (2) are the Fourier transforms of the corresponding coefficients in (1). For simplicity, we take the nearest-neighbour hopping:

$$E^{(cav)}(k) = -2t^{(cav)} \sum_r \cos(kr),$$

$$E^{(exc)}(k) = E_0 - 2t^{(exc)} \sum_r \cos(kr),$$

where $E_0$ is the offset between photonic and excitonic dispersion laws, and the summation is made on the nearest neighbours of zero point in the $r$-lattice.

4. Features of simulation
We note that the Rabi frequency in Eq. (2) plays the role of hopping between subsystems. The interparticle interaction term is diagonal allowing to use the Worm algorithm.
One can discuss the alternative approach including the diagonalization of the first three terms of the Hamiltonian (all the single-particle parts) and working in the basis of hybridized particles [10, 17]. This approach, however, has a certain disadvantage due to more complex form of the interaction term in the Hamiltonian.

The last remark applies to the terms with single operators (photon pumping and exciton decay). These terms generate kinks which add or remove particle from the worldline configuration, i.e. create worm ‘heads’ and ‘tails’. In the original Worm algorithm, these coefficients are added artificially and the count of worms is limited by algorithm. In our case, however, the worldline configuration may contain many worms simultaneously. The count of worms is determined by the actual model parameters (pumping intensity and lifetime of excitons) and temperature.

The example of the worldline configuration specific for the model (2) is shown in Figure 1.

Figure 1. The typical configuration of worldlines in simulation of polaritonic system (2) with diagrammatic QMC. The sites (placed vertically) correspond to two subsystems: excitons at the bottom (sites 0–7), photons at the top (sites 8–15). Particle worldlines (‘worms’) consist of horizontal lines (particle propagation in time), vertical changes (hopping), and worm ‘heads’ and ‘tails’ (circles). Width of the horizontal line shows the site occupation at the corresponding time range.

5. Calculation of average values
During the CTWL simulation, the average values are calculated. Mean energy $\langle E \rangle$ and average occupation numbers on sites $\langle n_i \rangle$ are obtained using standard averaging procedure [16]. To calculate occupation in momentum space $\langle n_k \rangle$, one needs to obtain also the Green function $\langle a_i^+ a_j \rangle$, and apply the Fourier transform $r \rightarrow k$. Calculation of more complex correlation function is straightforward.

6. Conclusion
To simulate the system of exciton polaritons described by the Hamiltonian (1), we developed a numerical calculation algorithm based on the modified Worm algorithm [15] of diagrammatic QMC [16]. The model parameters include Rabi splitting, dispersion laws of photons and excitons, and coupling to external field (optical pumping and exciton decay).
The algorithm allows to obtain mean energy, distribution of particles, and various correlation functions needed to study the state of the system. Numerical simulation of polaritonic system with various values of parameters would allow to find optimal parameters of the experiment, including the Bose-Einstein condensation of polaritons. The modifications of Worm algorithm are described in details.

Acknowledgments
P. F. Kartsev is grateful for support to Russian Foundation for Basic Research, Grant No. 15-02-02764.

References
[1] Lambert K. van Vugt et al. 2011 PNAS 108(2) 10050
[2] Rahimi-iman A et al. 2012 Phys. Rev. B 86 153308
[3] Sun Y and Wen P et al. 2017 Phys. Rev. Lett 118 016602
[4] Voronova N S and Lozovik Yu E 2012 Phys. Rev. B 86 193305
[5] Das A and Bhattacharya P et al. 2012 Phys. Rev. B 85 195321
[6] Amo A and Lefrere J et al. 2009 Nat. Phys. 5 805
[7] Bhattacharya A and Baten M Z et al. 2016 Phys. Rev. B 94 035203
[8] Lagoudakis K G and Ostatticky T et al. 2009 Science 326 974
[9] Colombelli R and Manceau J-M 2015 Phys. Rev. X 5 011031
[10] Takemura N and Anderson M D et al. 2016 Phys. Rev. B 94 195301
[11] Wouters V 2012 Phys. Rev. B 85 165303
[12] Verger A and Carusotto I and Ciuti C 2007 Phys. Rev. B 76 115324
[13] Wertz E and Amo A and Solnyshkov D D et al. 2012 Phys. Rev. Lett. 109 216404
[14] Yang Kai-Yu and Kozik E and Wang Xin and Troyer M 2011 Phys. Rev. B 83 214516
[15] Prokof’ev N V and Svistunov B V and Tupitsyn I S 1998 Phys. Lett. A 238 (4-5) 253
[16] Prokof’ev N V and Svistunov B V and Tupitsyn I S 1998 J. Exp. Theor. Phys. 87 310
[17] Berman O L and Lozovik Yu E and Snoke D W 2008 Phys. Rev. B 77 155317