Numerical simulation of polariton Bose gas thermalization

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Abstract. In this work, we present the numerical simulation of the process a Bose gas thermalization and the formation of the condensate. Our approach is based on kinetic equations and “Fermi’s golden rule” in the incoherent approximation. Direct summation of terms is performed using GPGPU OpenCL parallel code using AMD Radeon HD 7970.

1. Introduction
The problem of describing the evolution of a weakly interacting Bose gas (such as gas thermalization, i.e. relaxation to thermal equilibrium after a perturbation, or the formation of a Bose-Einstein condensate at lowering temperature) has received new applications recent years. First of all, they are (i) possible Bose condensation at room temperature for a system of exciton polaritons in semiconductor sample and (ii) the gamma-laser scheme based on annihilation of the Bose-condensed the positronium gas.

The evolution of weakly interacting Bose gas is essential to achieve Bose condensation in the polariton system in the semiconductor sample in the optical resonator under optical pumping [1]. This system is interesting because it can lead to the development of new optoelectronic devices and optical converters. The rate of a Bose condensate formation must prevail over the rate of decay of polaritons, as well as other losses. Due to experimental success, the system of exciton polaritons has become the object of intense theoretical [2], [3] and experimental [1] studies. The decisive role in the establishment of thermal equilibrium in this system is played by the interparticle interaction.

The proposed [4, 5] scheme of gamma-laser making use the annihilation of positronium atoms in the state of BEC, raises question of calculating the rates of all needed processes in the system, including thermalization and Bose condensate formation.

However, there are not many reliable theoretical works applying to these systems[6, 7]. To determine the optimal experimental parameters, it is necessary to build a reliable theoretical model of the system. In this work, we employ simple approach based on the “Fermi’s golden rule” and direct summation of kinetic terms.

2. Model
The basic model in the equilibrium statistical mechanics of the system is the case of low density and weak interaction. Let us consider the weakly interacting Bose gas with the contact interaction. The Hamiltonian of the system is
\[ \hat{H} = \hat{H}_0 + \hat{V} = \sum_k \varepsilon_k \hat{a}_k^\dagger \hat{a}_k + \sum_{k_1 k_2 k_3 k_4} U_{0_{k_1 k_2 k_3 k_4}} \hat{a}_{k_1}^\dagger \hat{a}_{k_2}^\dagger \hat{a}_{k_3} \hat{a}_{k_4} \]  

(1)

The prime at the summation sign denotes the momentum conservation law \((k_1 + k_2 = k_3 + k_4)\).

In the case of temperature high enough (i.e. no condensate) and incoherent limit (neglecting correlation of particle occupations) we can apply the “Fermi’s golden rule” for the relaxation time:

\[ \frac{1}{\tau} = \frac{2\pi}{\hbar} \sum_f |<i | \hat{V} | f>|^2 \delta(E_i - E_f) \]  

(2)

Thermalization dynamics of the system can be described by the quantum Boltzmann equation (QBE) taking into account the law of conservation of energy [8]. Thus a change of the particle density \(n_p\) is given by the equation:

\[ \frac{dn_p}{dt} = \frac{2\pi}{\hbar U_0^2} \sum_{qnm} \delta(\varepsilon_q + \varepsilon_p - \varepsilon_m - \varepsilon_n) \times \]  

\[ \times [(n_p + 1)(n_q + 1 + \delta_{pq})n_m(n_n - \delta_{nm}) - n_p(n_q - \delta_{pq})(n_m + 1)(n_n + 1 + \delta_{nm})] \]  

(3)

In further calculations we assume \(\frac{2\pi U_0^2}{\hbar} = 1\) and consider the dimensionless time.

3. Numerical calculation

Main obstacle to simulate the system evolution using Eq.(3) for reasonable system sizes \((L > 6.8)\) is caused by enormous amount of needed calculation. In our experience, it scales roughly as \(L^8\).

This required to apply the corresponding high-performance solution. In our work, we created a parallel GPGPU code using OpenCL language with acceptable resulting speed able to take as high as \(L = 12.18\). Our calculations were performed on the AMD Radeon HD 7970 graphic accelerator. Further acceleration is also possible, with the help of parallel computing and task distribution on multiple accelerators.

In Figs. 1,2,3,4 we present the results of simulation for the system \(L^3 = 12^3\) for several time slices in the time intervals of \(10^{-11}\) (dimensionless units). We plot the 2D momentum distribution for slice \(p_x = 0\), and additionally 1D slice for \(p_z = p_y = 0\).

We take different starting distributions of particles which reflect different temperatures \((T < T_c \text{ and } T > T_c)\, \text{Figs. 1 to 3})\) and shifted initial distributions due to e.g. optical pumping (Fig. 4).

All starting distributions were chosen as rectangular \((n_p = n_{max} \text{ at } |p| < \sigma)\) with small nonzero background \((n_p = n_{min} \text{ at } |p| \geq \sigma)\), which proven needed to get equilibration due to Umklapp processes.

All figures show reasonable behaviour. The systems reach expected thermal distribution.
Figure 1. The initial distribution of the particles (a) in three dimensional space 12x12x12 size gradually redistributed (b, c). The 2D slices on $p_z = 0$. Part (d) represents 1D slice on $p_y = p_z = 0$. We see the gradual change of distribution to equilibrium.
Figure 2. The initial distribution of the particles (a) in three dimensional space 12x12x12 size gradually redistributed (b,c,d). The case of lower temperature approaching $T_c$. 
Figure 3. The initial distribution of the particles (a) in three dimensional space 12x12x12 size gradually redistributed (b,c,d). The case of temperature lower than $T_c$. 
Figure 4. The initial distribution of the particles (a) in three dimensional space 12x12x12 size gradually redistributed (b,c,d). The case of shifted initial distribution modeling optical pumping of polaritons.
The figures clearly show the process of redistribution of occupation numbers, giving relaxation to thermal function and the beginning of the Bose condensate formation. In figure (1) the spread of the particles takes place over the entire space with a uniform increase in the occupation on all momenta, in contrast to the given initial filling. The case of a larger initial density in figure (2) corresponds to lower effective temperature of the system.

For figure (3) with even lower temperature we note the accumulation of particles in the center of the momentum space, reflecting beginning of the formation of Bose condensate.

4. Conclusion

We performed numerical simulation of the evolution of the particle distribution function in the incoherent approximation on the basis of kinetic equations and “Fermi golden rule” by direct calculation on a discrete momentum grid. The results of the calculations are presented as Figures 1 - 4, which show the evolution of particle distribution for different temperatures and starting occupations.

Such a direct numerical calculation of the Bose gas thermalization can be applied to determine optimal parameters of new BEC experiments with alkali gases and give new information on polaritonic condensation in the semiconductor sample under optical pumping.

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