Effective simulation of kinetic equations for bosonic system with two-particle interaction using OpenCL

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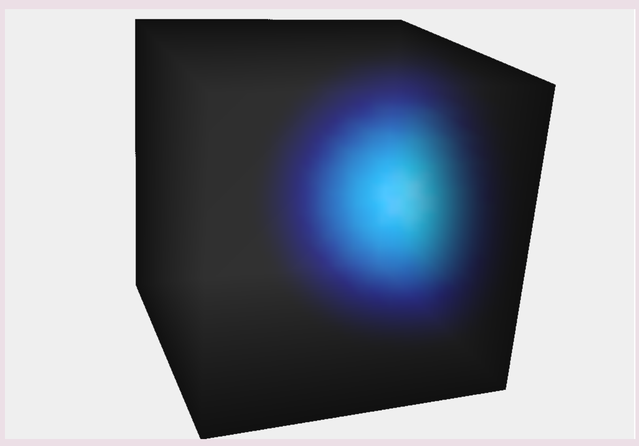
Physical system

One of the modern quantum systems attracting large interest is the gas of polaritons – quasiparticles in semiconductor under laser pumping in the optical resonator[1, 2, 3]. The interest to this system is caused by the possibility to achieve the unusual state of matter – the so-called Bose-Einstein condensate (BEC) – when large percent of particles occupy a single quantum state (are "condensed"). Unlike to more standard physical systems with BEC, such as superfluid helium and superconductors at cryogenic conditions, polaritonic condensation can be achieved at essentially higher temperatures, up to room temperature. This unique fact is explained by artificial nature of polaritons, as their effective mass and concentration can be controlled by the parameters of the experimental setup. As a result, this effect can form the basis for a new class of optoelectronic devices.

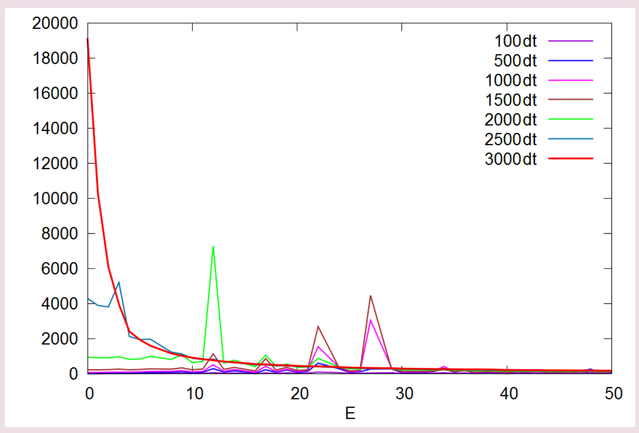
The main issue preventing successful demonstration of BEC in polaritons, is the small lifetime of polaritons not enough for the condensate to form. This sets the question which factors can determine the speed of condensate formation[4] or, at least reaching the thermal equilibrium (thermalization)[5]. To describe the experiment correctly, many effects should be taken into account, such as details of laser pumping, interparticle interaction and cooling by the thermal bath.

In this work, we present the effective algorithm to study the process of thermalization in the model system with two-particle interaction.

Sample results



Nonequilibrium distribution of particles ($n(\boldsymbol{k})$ at first stages of laser pumping: we see asymmetric distribution generated by beam



The evolution of particle distribution $f(E)$ shows relaxation to thermal equilibrium: zero energy becomes the most occupied.

References

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Model

Details of physical formulation can be found in [5]. In the system of free quantum particles (e.g. polaritons) contained in the finite volume a^3, the particles occupy the energy levels $\varepsilon_{\mathbf{k}} = \frac{\hbar^2}{2m}\mathbf{k}^2$, where $\hbar$ is the Planck constant, m is the particle mass, and momentum $\mathbf{k}$ is the 3D vector with components equal to discrete values with step $\frac{2\pi}{a}$. Later on, we use units such as $\varepsilon_{\mathbf{k}} = \mathbf{k}^2$ and k components are integer. For numerical study, the system is often discretized so that momentum is limited by some boundary value $-L/2 \le k_{x,y,z} < L/2$ with L low enough, i.e. 10,20,40,... *etc*. After that, the results are extrapolated to bulk limit.

Occupations of each momentum $\{n_{\mathbf{k}}\}$ give the particle distribution. One of the standard approaches to describe the time evolution of particle distribution, is the system of differential equations for $n_{\mathbf{k}}(t)$ – the so-called kinetic equations. In the case of contact interaction U_0 and temperature high enough, they are written as[5, 6]

$$\frac{dn_{\mathbf{1}}}{dt} = \frac{2\pi}{\hbar}U_0^2 \sum_{\mathbf{234}} [(n_{\mathbf{1}}+1)(n_{\mathbf{2}}+1+\delta_{\mathbf{12}})n_3(n_4-\delta_{\mathbf{34}}) - \tag{1}$$

$$-n_{\mathbf{1}}(n_{\mathbf{2}}-\delta_{\mathbf{12}})(n_{\mathbf{3}}+1)(n_4+1+\delta_{\mathbf{34}})]\delta_{\varepsilon_{\mathbf{1}}+\varepsilon_{\mathbf{2}},\varepsilon_{\mathbf{3}}+\varepsilon_4}\delta_{\mathbf{1}+\mathbf{2},\mathbf{3}+4},$$

where for simplicity we denote $\boldsymbol{k}_1$,...,$\boldsymbol{k}_4$ as $\mathbf{1}$,...,$\mathbf{4}$. The last Kronecker symbols δ are responsible for energy and momentum conservation laws, so actually this sum is only twofold with additional restriction. Later on we put $\frac{2\pi}{\hbar}U_0^2 = 1$.

This multiple sum is the main concern of our work. Amount of calculations for simple summation can be estimated as L^9. Simple CPU realization (Fortran + OpenMP) is practicly limited by $L = 12$ (several seconds each round of calculation).

Result in a nutshell

We use the analytic transformation (below) to get much better scaling $L^5 \log L$.
Simulation of systems as large as $L = 64$ becomes possible. For $L = 16$, each round of calculation (step of 4th order Runge-Kutta method) takes as low as 38ms on AMD Fury X (Fiji GPU). Such performance level allows to study the evolution of the system for prolonged time of up to 10^6 and more steps, to study weak effects and slow processes.

Benchmarks

System size is $L = 16$. Benchmark for several OpenCL devices. Seconds for 100 RK4 steps, the lower the better:

GPU Codename	NVidia GTX Titan Black (Kepler)	AMD Radeon HD 7970 (Tahiti)	AMD Radeon R9 Fury X (Fiji)	Intel CPU i7-4790 (Haswell)
FP64, seconds	10.1[a], 10.4[b]	6.32	3.75	151.4[c]
FP32, seconds	7.3[a], 7.8[b]	4.05	2.08	145.4
Specs: FP64, GFlop/s	1881[a], 941[b]	947	537.6	256
Memory bus, bit	384 bit	384 bit	4096 bit	64 bit
Memory bandwidth, GB/s	336	264	512	12.8 GB/s

[a] for DP/SP ratio 1/3, [b] for DP/SP ratio 1/6
[c] GFortran/OpenMP version took about 6 seconds per RK4 step, i.e. 4 times slower though we could not reach 100% CPU utilization

Analytic transformation

Let us introduce the variables $n_{\mathbf{k}\varepsilon} = n_{\mathbf{k}}\delta_{\varepsilon,\varepsilon_{\mathbf{k}}}$ in the extended 4D space $(\mathbf{k}, \varepsilon)$. Then we can write typical term of Eq. (1) as

$$\sum_{\boldsymbol{k}_2\boldsymbol{k}_3\boldsymbol{k}_4\varepsilon_2\varepsilon_3\varepsilon_4} \tilde{n}_{\boldsymbol{k}_1\varepsilon_1}\tilde{n}_{\boldsymbol{k}_2\varepsilon_2}n_{\boldsymbol{k}_3\varepsilon_3}n_{\boldsymbol{k}_4\varepsilon_4}\delta_{\varepsilon_4,\varepsilon_1+\varepsilon_2-\varepsilon_3}\delta_{\boldsymbol{k}_4,\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3},$$

where we set $\tilde{n}_{\boldsymbol{k}\varepsilon} = n_{\boldsymbol{k}\varepsilon} + 1$.
This multiple sum can be understood as a discrete convolution and therefore easily transformed to single sum by applying the Fourier transform $\boldsymbol{k}, \varepsilon \to \boldsymbol{r}, \gamma$ and the Convolution theorem[7].
Then after some analytical work, the Equation (1) becomes

$$\frac{dn_{\boldsymbol{k},\varepsilon}}{dt} = \tilde{n}_{\boldsymbol{k},\varepsilon}\left(\alpha_{\boldsymbol{k},\varepsilon} + \beta_{2\boldsymbol{k},2\varepsilon} - n_{\boldsymbol{k}+\frac{L}{2},\varepsilon}\right) - n_{\boldsymbol{k},\varepsilon}\left(\tilde{\alpha}_{\boldsymbol{k},\varepsilon} + \tilde{\beta}_{2\boldsymbol{k},2\varepsilon} - \tilde{n}_{\boldsymbol{k}+\frac{L}{2},\varepsilon}\right), \tag{2}$$

where

$$\alpha_{\boldsymbol{r},\gamma} = V^2 n^2_{\boldsymbol{r},\gamma}\tilde{n}_{-\boldsymbol{r},-\gamma} - V n_{2\boldsymbol{r},2\gamma}n_{-\boldsymbol{r},-\gamma}, \qquad \beta_{\boldsymbol{r},\gamma} = V n^2_{\boldsymbol{r},\gamma}, \tag{3}$$

$$\tilde{\alpha}_{\boldsymbol{r},\gamma} = V^2 \tilde{n}^2_{\boldsymbol{r},\gamma}n_{-\boldsymbol{r},-\gamma} + V \tilde{n}_{2\boldsymbol{r},2\gamma}\tilde{n}_{-\boldsymbol{r},-\gamma}, \qquad \tilde{\beta}_{\boldsymbol{r},\gamma} = -V\tilde{n}^2_{\boldsymbol{r},\gamma}$$

are the Fourier transforms of the corresponding $\alpha_{\boldsymbol{k},\varepsilon}$, $\tilde{\alpha}_{\boldsymbol{k},\varepsilon}$, $\beta_{\boldsymbol{k},\varepsilon}$, $\tilde{\beta}_{\boldsymbol{k},\varepsilon}$. Index $\boldsymbol{k} + \frac{L}{2}$ denotes summation on all $\boldsymbol{k}' = \boldsymbol{k} + \boldsymbol{q}$ such that the components of $2\boldsymbol{q}$ are either zero or equal to $\pm L$. The derivation is not shown but straightforward.

Volume of the 4D lattice used in the Fourier transform is $V = L^3 E_{\max} \sim L^5$, where $E_{\max} = 2L^2 \ge 2 \cdot 3\left(\frac{L}{2}\right)^2$ taken to be at least twice the maximal energy of single particle, to get rid of extra terms after convolution. For example, $L = 16$ gives $E_{\max} = 512$ best suited for radix-2 FFT.