Simulation of the weakly interacting Bose gas relaxation for cases of various interaction types

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Abstract.
In this work, we investigate the role of interactions in the process of thermalization of a weakly interacting Bose gas. The system of kinetic equations based on the ‘Fermi’s golden rule’ is solved numerically using special transformation for calculation efficiency. We study the distribution function for particles in various conditions, including interaction with phonon subsystem, i.e. energy exchange with thermal bath. The possibility to achieve the state of Bose-Einstein condensation with specific values of parameters, is also discussed.

1. Introduction
The phenomenon of Bose Einstein condensation (BEC) in various experimental systems attracts constant attention. Some of the new experiments are based on the study of the evolution of the Bose gas [1, 2] and Bose Einstein condensate [3]. Both experimental [4] and theoretical [5] works on the evolution of the Bose gas in various formulations of the problem are carried out.

It is a particular problem to determine the optimal parameters of the experiment with Bose gas, including that of achieving the state of BEC[6]. Among the processes determining the system evolution we distinguish the phenomenon of thermalization, i.e. relaxation to thermal equilibrium after perturbation. Thermalization is important for reaching BEC in many promising Bose systems, such as the cold gas of alkali atoms in an optical trap [7], exciton polaritons in a semiconductor resonator [8, 9], and probably for positronium gas in the recently proposed gamma laser scheme[10, 11].

The evolution of the many-particle system is governed by the interactions. The two-particle interaction affects the rate of thermalization in the system (as well as the spectrum of excitations of the system [12]), while the interaction with the phonon subsystem is important for energy exchange with the environment. To describe the behaviour of a complex interacting system, it is necessary to build a reliable theoretical model which takes into account all the important parameters of the problem and the interactions present in the system.

In this paper, we study numerically the effects of these two types of interaction on the relaxation characteristics in the weakly-interacting Bose gas. Successful simulation of many-particle kinetics would help to visualize important processes, and to plan further study.

2. Model
First, let us write the Hamiltonian of the weakly-interacting Bose gas of e.g. excitons ($\hat{a}, \hat{a}^\dagger$) coupled with phonon subsystem ($\hat{b}, \hat{b}^\dagger$):
\[ \hat{H} = \sum_k \varepsilon_k \hat{a}_k^\dagger \hat{a}_k + \sum_q \varepsilon_q \hat{b}_q^\dagger \hat{b}_q + \sum_{k_1 k_2 k_3 k_4} U_{k_1 k_2 k_3 k_4} \hat{a}_{k_1}^\dagger \hat{a}_{k_2}^\dagger \hat{a}_{k_3} \hat{a}_{k_4} + \sum_{k q} M_{k q} \hat{a}_k^\dagger \hat{a}_{k-q} + H.c. \]  

(1)

Here \( \varepsilon_k \) and \( \tilde{\varepsilon}_q \) are the dispersions laws of excitons and phonons, \( U_{k_1 k_2 k_3 k_4} \) is the two-particle interaction and \( M_{k q} \) describes the particle transition with creation or annihilation of phonon. For the sake of simplicity, we restrict ourselves to the case of contact interaction \( U_{k_1 k_2 k_3 k_4} \equiv U_0 \delta_{k_1+k_2,k_3+k_4} \) and constant matrix element \( M_{k q} \equiv M_0 \).

The phonon subsystem is considered as external bath with fixed temperature \( T^{(bath)} \) and classical field \( \langle b_q \rangle \simeq \sqrt{n^{(phon)}(\tilde{\varepsilon}_q)} \), \( \langle b_q^\dagger \rangle \simeq \sqrt{n^{(phon)}(\tilde{\varepsilon}_q) + 1} \), with \( \tilde{n}^{(phon)}(\tilde{\varepsilon}) = \frac{1}{\epsilon^{(phon)}(\tilde{\varepsilon})} \).

Then we study the kinetics of the main subsystem (e.g. excitons) only.

The evolution of bosonic system at high enough temperature can be described by the Boltzmann equation[12, 13]. Kinetic equation for the specific occupation number \( n_k \) is generated by the ‘Fermi’s golden rule’ giving the rate of changes

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

(2)

where \( |i\rangle \) and \( |f\rangle \) are initial and final states of the quantum system connected by the perturbation operator \( \hat{V} \) changing the occupation number \( n_k \), with the conservation of the full system energy \( E_i = E_f \). Later on, we assume dimensionless time and choose unities so that \( \frac{2\pi}{\hbar} \equiv 1 \).

In thermal equilibrium, occupation numbers are given by Bose-Einstein distribution function. If the stable state is disturbed, the occupations tend to relax and return to the equilibrium[14]. For small deviations from the equilibrium, the rate of relaxation should be proportional to \( \langle V \rangle^2 \).

The numerical simulation of kinetic equations can be done using any appropriate method. We simulate the evolution of the occupation numbers described by the system of kinetic equations using the especially developed numerical algorithm[14]. The main difficulty in the simulation is caused by the amount of calculations increasing drastically with the size of system and can be partially overcome using the auxiliary analytic transformation[15].

Let us consider the terms generated by interactions in (1).

**Two-particle interaction.** To calculate matrix elements, we need to neglect correlations between occupation numbers: \( \langle n_p n_q \rangle = \langle n_p \rangle \langle n_q \rangle \), assuming the temperature be high enough (far from condensation temperature \( T_c \)). Then the equation (2) gives

\[ \frac{dn_k^{(e-o)}}{dt} = \frac{2\pi}{\hbar} U_0^2 \sum_{p \ge q} \{(n_1 + 1)(n_2 + 1 + \delta_{12})n_3(n_4 - \delta_{34}) - 
- n_1(n_2 - \delta_{12})(n_3 + 1)(n_4 + 1 + \delta_{34})\} \delta(\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4). \]

(3)

Here we denoted \( k_1, \ldots, k_4 \) as 1, . . . , 4. The Kronecker symbols \( \delta_{12}, \delta_{34} \) help to account the case of coinciding momenta of Bose particles.

Considering the nonlinear nature of two-particle interaction, the relaxation rate can be estimated as \( \frac{1}{\tau} \simeq U_0^2 N^2 \), with \( N \) the count of Bose particles.

**Interaction with phonon bath.** To take into account the finite width of phonon levels \( \Gamma \), we introduce the Gaussian form factor \( F(\Delta E) \sim \exp(-\langle \Delta E/\Gamma \rangle^2) \):
due to phonon field, can be estimated as  
\[
\frac{dP^{(\text{e-ph})}}{dt} = P^{(+)} - P^{(-)},
\]

where 
\[
P^{(+)} = M_0^2 \sum_q [(n_{k+1}) n_{k-q} \{ (n_{E}^{(\text{phon})} + 1) F(\varepsilon_k - \varepsilon_{k-q} + \tilde{\varepsilon}_q) - n_{E}^{(\text{phon})} F(\varepsilon_k - \varepsilon_{k-q} - \tilde{\varepsilon}_q) \}],
\]

\[
P^{(-)} = M_0^2 \sum_q [n_k (n_{k-q} + 1) \{ n_{E}^{(\text{phon})} F(\varepsilon_k - \varepsilon_{k-q} + \tilde{\varepsilon}_q) - (n_{E}^{(\text{phon})} + 1) F(\varepsilon_k - \varepsilon_{k-q} - \tilde{\varepsilon}_q) \}].
\]

Notice the two terms in both branches of particle addition and removal. The relaxation rate due to phonon field, can be estimated as \( \frac{1}{\tau} \sim M_0^2 \) (independent of \( N \)).

3. Results of numerical simulation

We investigate the effects of interparticle interaction and interaction with thermal bath separately. In both cases we expect that the excitation would decay and the state approaches thermal equilibrium. In the case of exponential decay, we try to extract its time constant \( \tau \).

As a starting (excited) state, we use the following particle distribution:

\[
\begin{cases}
n_{k_{\text{(start)}}}^{(\text{inside})} = N^{(\text{inside})}, & |k - k_0| < R, \\
n_{k_{\text{(start)}}}^{(\text{outside})} = N^{(\text{outside})}, & |k - k_0| \geq R,
\end{cases}
\]

where \( R \) is the size of initial “droplet” in momentum space, centered in the point \( k_0 \).

The simulations were carried for the system of size \( L^3 = 16^3 \) with dimensionless time step \( \Delta t = 10^{-11} \). The problem parameters were taken \( c = 1.0, \Gamma = 3.0, R^2 = 6.0, N^{(\text{inside})} = N^{(\text{outside})}/100 \). The units were chosen so that dispersion laws were \( \varepsilon_k = n_x^2 + n_y^2 + n_z^2 \), \( \tilde{\varepsilon}_q = c \sqrt{n_x^2 + n_y^2 + n_z^2} \) with \( n_\alpha \) integer \((-L/2 \leq n_\alpha < L/2)\). The number of time steps needed for relaxation, did not exceed the value of \( 3 \cdot 10^5 \). The size \( L = 16 \) is large enough to see the needed behaviour.

Two-particle interaction. First, we put \( U_0 = 1, M_0 = 0 \). In Fig.1(a) we see how particle distribution changes in time. To confirm the Bose-Einstein form of the final distribution, we introduce the characteristic function \( L(E) \equiv \ln \left[ 1 + \frac{1}{4T(E)} \right] \), which equals to \((E - \mu)/k_BT\) in the case of Bose-Einstein function. In Fig.1(b), we see the tendency of \( L(E) \) to become linear, confirming the fact that the system approaches the thermal distribution.

In Fig. 2(a), we show the temperature calculated by fitting the characteristic function with linear function in the range \( E = 40..120 \). Note that the final value of \( k_BT \) is reached very quickly. In Fig. 2(b), we show the mean squared deviation of \( L(E) \) from the linear function decreasing to values as low as \( 10^{-11} \), for \( N = 50 \, 000 \). The characteristic time of relaxation \( \tau \) depending on \( N \), is plotted in Fig. 3. The power law is almost \( N^{-2} \) as we expected.

So, for the thermalization due to interparticle interaction, we can see the following stages: (i) fast thermalization of particles in the middle range of energies; (ii) the temperature approaches the final value determined by full energy of the system; (iii) the range of energies where particles follow the thermal law, expands to all energies.

Interaction with phonon bath. Second, we put \( U_0 = 0, M_0 = 10^3 \). In Fig. 4 we show the graphs of \( f(E) \) and \( L(E) \) calculated for \( N = 10^5 \). The distribution approaches thermal function again, though the stages are slightly different: (i) fast thermalization of particles in the limited range of energies; (ii) the temperature decreases to the final value determined by the bath \( T \to T^{(\text{bath})} \).
Figure 1. (a) Typical evolution of the particle distribution function \( f(E) = n(E)/g(E) \) from the initial nonequilibrium state (5), calculated for \( N = 5 \cdot 10^4, U_0 = 1 \), in the case of two-particle interaction. Initially flat, the distribution transforms to emphasized peak at nonzero energy, which then shifts to \( E = 0 \). Time \( t = 1 \cdot 10^{-6} \) appears enough to reach the Bose-Einstein function. (b) Evolution of the characteristic \( L(E) \) calculated for data in Fig. 1(a). Notice the limited range of linear behaviour and gradual change of the slope \( \sim 1/k_B T \). The range of linear behaviour starts from \( E \simeq 40..120 \) and slowly extends to all energy range. At the (dimensionless) time \( t = 3 \cdot 10^{-6} \), the graph becomes very close to a linear law.

Figure 2. (a) Time dependence of the temperature calculated for data in Fig. 1(a). (b) Mean squared deviation of \( L(E) \) from the linear law, calculated in the range \( E = 40..120 \), depending on time \( t \). Minimal value is limited by \( \sim 10^{-11} \) due to precision of numerical algorithm.
Figure 3. Characteristic time $\tau$ to establish equilibrium depending on the total number of particles $N$. Dots are the experimental data, the line shows the power-law fit. The power index -1.86 is close to expected -2. Relative error of $\tau$ is close to $\sim 5 \cdot 10^{-2}$.

$f(E)=\frac{n(E)}{g(E)}$

$\ln(1+1/f(E)) \approx (E - \mu)/kT$

Figure 4. (a) Evolution of the particle distribution function in the case of interaction with phonon subsystem only, calculated for $N = 10^5$. (b) Evolution of the characteristic function $L(E)$ calculated for $N = 4.8 \cdot 10^4$.

simultaneously with expanding the range of energies. In our calculation, the time of calculation $t_{(max)} = 10^{-5}$ ($10^6$ time steps) was not enough to reach the completely linear law. Though the details can be different for various parameters of the phonon spectra, the characteristic time is determined by the exciton-phonon matrix element $M_0$ and does not depend on the number of particles $N$.

4. Conclusion
We studied the features of weakly-interacting Bose gas thermalization due to interparticle interaction and interaction with phonon subsystem. While the cooling of the gas can be realized
only with energy exchange with bath, internal redistribution and relaxation is more efficient with two-particle interaction. Both mechanisms should be taken into account when planning the experiments on cooling and condensation in novel Bose systems. The thermalization occurs in several stages, first in restricted range of energies, then the area of equilibrium is extended to wider range of energies.

The numerical algorithm [15] allows to simulate the kinetics of the finite-size interacting Bose systems, in particular the process of thermalization. In study of more complex systems for which the selection of optimal parameters for establishing equilibrium can be quite difficult, numerical simulation of this process is a promising direction of research.

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References

[1] Banuls M C, Cirac J I and Hasting M B 2011 Phys. Rev. Lett. 106 050405
[2] Lin Ch-J and Motrunich Oi I 2017 Phys. Rev. A 95 023621
[3] Berman O L, Gumbs G and Kezerashvili R Ya 2017 Phys. Rev. B 96 014505
[4] Das A, Bhattacharya P, Banerjee A and Jankowski M 2012 Phys. Rev. B 85 195321
[5] Wertz E, Amo A, Solnyshkov D D, Ferrier L, Liew T C H, Sanvitto D, Senellart P, Sagnes I, Lemaitre A, Kavokin A V, Malpuech G and Bloch J 2012 Phys. Rev. Lett. 109 216404
[6] Straatsma C J E, Colussi V E, Davis M J, Lobser D S, Holland M J, Anderson D Z, Lewandowski H J and Cornell E A 2016 Phys. Rev. A 94 043640
[7] Sturm M R, Schlosser M, Walser R and Birkl G 2017 Phys. Rev. A 95 063625
[8] Voronova N S, Kazakov Y E 2012 Phys. Rev. B 86 195305
[9] Cho Ch-H, Nukala P, Lambert K, Piccione A and Agarwal R 2011 PNAS 108 10050
[10] Avetissian H K, Avetissian A K and Mkrchian G F 2014 Phys. Rev. Lett. 113 023904
[11] Wang Yi-Hs, Anderson B M and Clark Ch W 2014 Phys. Rev. A 89 043624
[12] Griffin A, Nikuni T and Zaremba E 2009 Bose-condensed gases at finite temperatures (Cambridge: Cambridge University Press)
[13] Davis M J, Ballagh R J and Burnett K 2001 J. Phys. B: Atomic, Molecular and Optical Physics 34 4487
[14] Kartsev P F, Kuznetsov O I 2016 J. Phys.: Conf. Ser. 737 012033
[15] Kartsev P F 2017 Proc. of the 5th Int. Workshop on OpenCL (New York: USA/ACM) Article No. 28