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BTELab, a MATLAB Programme Code for solving Quantum Boltzmann Transport Equation with all Collision Terms within Trapping Potential

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Abstract

This paper presents Quantum Boltzmann Transport Equation Laboratory (QBTELab), an advanced easy-to-use toolbox to solve many complex problems related to Bose-Einstein Condensate (BEC). The model equation that BTELab solves is the Quantum Boltzmann Transport Equation (QBTE) with all collision terms within trapping potential. Inelastic scattering (Exciton-phonon collision), elastic scattering (exciton-exciton collision), Auger decay and radiative non-radiative decay are included here as the collision terms. The programme code has been written in MATLAB. From the results it can be said that the programme is working properly and it has enough numerical stability.

The aim of this paper is to provide programme code to solve the full QBTE. QBTE is a powerful tool for investigating the transport phenomena in various systems like semiconductors, plasmas, nuclear reactors, heat transfer process, fluid dynamics etc and specially different problems related to BEC.

Keywords: Quantum Boltzmann Transport Equation Laboratory (QBTELab), MATLAB programme code to solve Quantum Boltzmann Transport Equation with all collision term, Bose-Einstein Condensate, Numerical solution of three dimensional Quantum Boltzmann Transport Equation

1.Introduction

The idea of Bose-Einstein Condensate (BEC) was given by Satyendra Nath Bose and Albert Einstein in 1925. First BEC was created experimentally in 1995. After that, lot of theoretical and experimental work has been done in this field.

Theoretically to see the relaxation kinetics and Bose-Einstein Condensation, researchers used the Boltzmann Transport equation (BTE) and Gross–Pitaevskii equation. Here the programme code of the full BTE (BTELab) has been given and solved including exciton-phonon collision, exciton-exciton collision, radiative nonradiative decay and Auger decay using MATLAB.

A mathematician and theoretical physicist Ludwig Boltzmann developed the BTE in 1872[1].The statistical behaviour of a non-equilibrium thermodynamic system can be explained by using this equation. It is a fundamental tool to understand how particles move with energy and momentum through a system. The Boltzmann equation is a nonlinear equation. Here the unknown function is the probability density function. It describes the probability distribution of particles for the position and momentum within a six-dimensional space. To solve the various forms of the Boltzmann equation, generally numerical methods are used.

BTE is used to study the transport phenomena in nuclear reactor physics like neutron flux and power distribution within a nuclear reactor. In heat transfer it helps to understand conductive, convective and radiative heat transfer by modelling the movement of energy. It can also be applied to study fluid dynamics like viscosity, thermal conductivity and electrical conductivity. In plasma physics it is used to describe particle in gas discharges, and calculate electron energy distribution function in plasmas. BTE is used to study electron transport in semiconductors. It is helpful to analyse material properties and can investigate how a non-equilibrium system goes towards equilibrium.

The kinetic theory of gasses, phonon transport in superfluid, radiative transfer in planetary and stellar atmospheres, electron transport in solids and plasmas, neutron transport in nuclear reactors etc can be studied by using the Boltzmann equation. When a fluid is in motion, the Boltzmann equation can be used to calculate the change of heat energy and momentum and other properties of fluids such as viscosity, thermal conductivity, and electrical conductivity. Nowadays the movement of cells [2, 3] can be determined by using the Boltzmann equation. This equation can be used to explain invasions of cancer cells in tissues, morphogenesis, and chemo taxis-related effects.

The three-dimensional linearized BTE only for phonons has been solved by the researchers of reference [4] using variance reduced Monte Carlo approach. The nonlinear Boltzmann equation for the homogeneous isotropic case has been solved using MATLAB program by the researcher of reference [5]. HOMISBOLTZ, an open-source program was presented by them to deal with different applications in thermodynamics, econo-physics and socio dynamics. The researcher of reference [6] solved the collision term in the time dependent Boltzmann equation numerically for the application to a simple 2D system. The evolution of a

homogeneous gluon system and possibilities of condensation have been studied by the researcher of reference [7] by using the Relativistic Boltzmann-Nordheim (RBN) transport approach that includes the quantum effects of Bose-Einstein Statistics.

The researcher of reference [8] used an ab initio transport model to calculate the electrical mobility and Seebeck coefficient of n-type semiconductors using the Boltzmann transport equation including elastic scattering and inelastic scattering, but not three dimensional. BTE has been used for nano-scale thermal analysis by the researchers of reference [9]. In this case researchers used Fast Fourier Transform (FFT) based algorithm to solve BTE for phonon scattering which reduced the computational time significantly. The researchers of reference [10] reviewed the various modelling approaches of BTE. An algorithm of the linear BTE has been developed to model a photon beam data and solved numerically by the researchers of reference [11].In this case the authors assumes that radiation particles only interact with the matter but not with each other and it is valid for the case where no external magnetic field is present. The researchers of reference [12] model nanoscale heat conduction by using the discrete form of Boltzmann transport equation. A utility computable model of the Boltzmann equation for bimolecular chemical reactions was presented by the reference [13] to determine how chemical reactions affect kinetic theory. But till now the three-dimensional, full Boltzmann transport equation with all collision term including elastic scattering (exciton-exciton collision) and inelastic scattering (exciton-phonon collision), Auger decay and radiative non-radiative decay has not been solved. In this case excitons are within a potential trap and it is possible to add or remove any collision term from the programming according to the requirement.

In reference [3], the researchers solved the two-dimensional BTE numerically but, in their work, it has been mentioned that if it has been solved in three dimensions then it would be more realistic. In this case researchers of reference [3] can use our MATLAB programming code that can solve three dimensional BTE.

The goal of this work is twofold:

(i) Solve the full BTE including all collision terms to see the full relaxation kinetics and BEC of excitons.
(ii) Distribute an open-source programme for dealing with different other problems.

This paper is organised as follows: In section 2, the numerical modelling of the BTE has been discussed. The description of the MATLAB programme code has been given in section 3. The procedure of using MATLAB programme code QBTELab has been discussed in section 4. In section 5, results have been presented. Finally, section 6 is a short summary of the work.

2. Applications

The Quantum Boltzmann Transport Equation with all collision terms within trapping potential has many applications in research. These are

(i) Condensed Matter Dynamics: In this case it studies quantum many bodies collision and transport in dense and correlated systems where the full collision in and collision out terms are necessary to describe the evolution of the system.

(ii) Plasma Physics: In the case of relativistic heavy ion collision QBTE is used to describe the evolution of quark gluon plasma. Elastic and inelastic collisions both are necessary for this study.

(iii) Semiconductor nano-electronics: For the study of Metal-Oxide-Semiconductor Field-Effect Transistor (MOSFET), quantum dots i.e. high field, non-equilibrium electron transport in nanometre scale device, the full collision term needed to replace the relaxation time approximation with rigorous scattering rates.

(iv) Collective Modes and Hydrodynamics: In the case of harmonically trapped quantum gasses, for example Bose Einstein condensate and superfluid fermions, the QBTE is used to study hydrodynamic expansion, collective oscillation and damping.

(v) Inelastic Collisions and Two Body Loss: In the trapped molecular gasses, the inelastic quantum Boltzmann equation is used to analyse particle loss and temperature evolution.

(vi) Non-Equilibrium Dynamics and thermalization: The QBTE is used to study about thermalization behaviour of non-equilibrium quantum gasses.

(vii) Spin transport and relaxation: For the spin polarized Fermi gasses the QBTE is used to study spin wave damping and the transport of spin component.

(viii) Quantum simulation of Transport: Under non-uniform velocity fields the QBTE is used on trapped-ion quantum computers to simulate fluid dynamics, including advection-diffusion.

3.Full Boltzmann Transport Equation with its Numerical Modelling

The BTE,[14] relates the particles occupation number Ψ as a function of radius r, momentum ħk and time t, is given by

$$\frac{\partial \Psi}{\partial t} + \left(\vec{v} \cdot \overrightarrow{\nabla_r}\Psi + \vec{F} \cdot \frac{1}{\hbar}\overrightarrow{\nabla_k}\Psi\right)_{drift+force} = \left(\frac{\partial \Psi}{\partial t}\right)_{\text{coll+int}} \quad \ldots\ldots\ldots\ldots\ldots (1)$$

The second two terms are known as drift and force term. Where v is velocity, F is force, $\overrightarrow{\nabla_r}$ is nabla operator in r space and $\overrightarrow{\nabla_k}$ is nabla operator in k space. Right hand side term is known as collision and interaction term. The collision and interaction terms are exciton-phonon collision, exciton-exciton collision, Auger decay, radiative decay and non-radiative decay. Therefore, the full BTE is

$$\frac{\partial \Psi}{\partial t} + \left(\vec{v} \cdot \overrightarrow{\nabla_r}\Psi + \vec{F} \cdot \frac{1}{\hbar}\overrightarrow{\nabla_k}\Psi\right)_{drift+force} = \left(\frac{\partial \Psi}{\partial t}\right)_{\text{phonon-collision}} + \left(\frac{\partial \Psi}{\partial t}\right)_{\text{exciton-exciton-collision}} + \left(\frac{\partial \Psi}{\partial t}\right)_{\text{AG-decay}} + \left(\frac{\partial \Psi}{\partial t}\right)_{\text{R-nr-decay}} \quad \text{..... (2)}$$

If we put drift and force term on the right-hand side we get

$$\frac{\partial \Psi}{\partial t} = \left(\frac{\partial \Psi}{\partial t}\right)_{\text{phonon-collision}} + \left(\frac{\partial \Psi}{\partial t}\right)_{\text{exciton-exciton-collision}} + \left(\frac{\partial \Psi}{\partial t}\right)_{\text{AG-decay}} + \left(\frac{\partial \Psi}{\partial t}\right)_{\text{R-nr-decay}} - \left(\vec{v} \cdot \overrightarrow{\nabla_r}\Psi + \vec{F} \cdot \frac{1}{\hbar}\overrightarrow{\nabla_k}\Psi\right)_{drift+force} \quad \text{..... (3)}$$

3.1 Drift and Force terms of the Boltzmann equation

$$\frac{\partial \Psi}{\partial t} = -\vec{v}.\overrightarrow{\nabla_{\mathrm{r}}}\Psi - \vec{\mathrm{F}}.\frac{1}{\hbar}\vec{\nabla} \times \Psi \quad \text{..... (4)}$$

Here, the potential trap has been created by using the potential in the force term. As we know the force $F = -\frac{\partial V}{\partial r}$ and the potential $V(\vec{r}) = c\vec{r}^2$ has been used here. Therefore, $\vec{F} = -2cr$, where c is steepness constant. The velocity $\vec{v} = \frac{\hbar\vec{k}}{M_x}$, with the effective mass M_x and momentum vector $\vec{k}$.Therefore, the equation (4) can be written as

$$\frac{\partial \Psi}{\partial t} = -\left(\frac{\hbar k}{M_x}\right).\frac{\partial \Psi}{\partial r} + \left(\frac{2cr}{\hbar}\right).\frac{\partial \Psi}{\partial k} \quad \text{..... (5)}$$

3.1.1 Numerical Modelling

By using the finite difference method this equation has been discretized in the following way

$$\frac{\partial \Psi}{\partial r} = \frac{\Psi_j - \Psi_{j-1}}{\Delta r} \quad with\, r = r_0 \dots \dots \dots r_j \;\; and\; r_j = j\Delta r \qquad \dots\dots\dots\dots\dots (6)$$

$$\frac{\partial \Psi}{\partial k} = \frac{\Psi_l - \Psi_{l-1}}{\Delta k} \quad with\, k = k_0 \dots \dots \dots k_l \;\; and\; k_l = l\Delta k \qquad \dots\dots\dots\dots\dots (7)$$

Here, j and $l$are any integer.

Using $k^2 = \frac{2M_x\xi}{\hbar^2}, \xi_l = \Delta\xi.\, l,\;\; \Delta\xi = \frac{\xi_0}{m}\; and\; \xi_0 = 2M_x v_s^2$(where ξ is energy) the equation can be written as

$$\left(\frac{\partial \Psi}{\partial t}\right)_{Drift\&Force} = -\left(\frac{2v_s}{m^{\frac{1}{2}}.\Delta r}\right)\left[l^{\frac{1}{2}}\{\Psi(j,l) - \Psi(j-1,l)\}\right] + \left(\frac{2c\Delta r m^{1/2}}{M_x v_s}\right)\left[jl^{1/2}\{\Psi(j,l+1) - \Psi(j,l)\}\right] \dots\dots\dots\dots\dots (8)$$

3.2 Exciton Phonon Collision

Exciton phonon collision term of the Boltzmann equation is given by [15]

$$\left(\frac{\partial \Psi_{\vec{k}}}{\partial t}\right)_{ex_ph} = -\frac{2\pi}{\hbar}\sum_{\vec{p}}\left|M_{x-ph}(\vec{p}-\vec{k})\right|^2 \times [\{\Psi_{\vec{k}}(1+n^{ph}_{\vec{k}-\vec{p}})(1+\Psi_{\vec{p}}) - (1+\Psi_{\vec{k}})n^{ph}_{\vec{k}-\vec{p}}\Psi_{\vec{p}}\}\delta(\xi_{\vec{k}} - \xi_{\vec{p}} - \hbar\omega_{\vec{k}-\vec{p}}) + \{\Psi_{\vec{k}} n^{ph}_{\vec{p}-\vec{k}}\left(1+\Psi_{\vec{p}}\right) - \left(1+\Psi_{\vec{k}}\right)\left(1+n^{ph}_{\vec{p}-\vec{k}}\right)\Psi_{\vec{p}}\} \times \delta(\xi_{\vec{k}} - \xi_{\vec{p}} + \hbar\omega_{\vec{p}-\vec{k}})] \dots\dots\dots\dots\dots (9)$$

Here, $\left|M_{x-ph}(\vec{p}-\vec{k})\right|^2 = (\hbar D^2\left|\vec{p}-\vec{k}\right|)/(2V\rho v_s)$ represents the exciton phonon coupling between two momentum state $\vec{p}$ and $\vec{k}$with D is the deformation potential energy, the crystal volume V, the crystal densityρ and the sound velocityv_s. $\Psi_{\vec{p}}$ and $\Psi_{\vec{k}}$ are exciton occupation number in $\vec{p}$ state and $\vec{k}$ state respectively. Phonon occupation number

$n^{ph}_{\vec{p}-\vec{k}} = 1/\left[\exp\left(\frac{\hbar\omega_{\vec{p}-\vec{k}}}{k_B T_{bath}}\right)-1\right]$, exciton energy in $\vec{k}$ state $\xi_{\vec{k}} = \frac{\hbar^2\boldsymbol{k^2}}{\boldsymbol{2M_x}}$, exciton energy in $\vec{p}$ state $\xi_{\vec{p}} = \frac{\hbar^2\boldsymbol{p^2}}{\boldsymbol{2M_x}}$and phononenergy$\hbar\omega_{\vec{k}-\vec{p}} = \hbar v_s\left|\vec{p}-\vec{k}\right|$. The details are given in the reference [10].

Now to calculate numerically, the exciton phonon collision equation has been transferred from momentum space to one dimensional energy space by using the equation

$$\frac{\partial\Psi_\xi}{\partial t} = \frac{V}{(2\pi)^3}\int_0^\pi sin\,\theta\, d\theta \int_0^{2\pi} d\varphi \int_0^\infty k^2 \frac{\partial\Psi_{\vec{k}}}{\partial t} dk \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (10)$$

Converting all k terms into energy term with $\xi = \frac{\hbar^2k^2}{2M_x}$ and $\xi_1 = \frac{\hbar^2p^2}{2M_x}$ we get

$$\left(\frac{\partial\Psi_\xi}{\partial t}\right)_{ex-ph} = -\frac{\mathrm{C}_1}{\sqrt{\xi}}\int_0^\infty (\xi-\xi_1)^2 \times [\{\Psi_\xi(1+n^{ph}_{\xi-\xi_1})(1+\Psi_{\xi_1}) - (1+\Psi_\xi)n^{ph}_{\xi-\xi_1}\Psi_{\xi_1}\}$$

$\times H\left(Q_s - \sqrt{\xi}+\sqrt{\xi_1}\right)\times H\left(-Q_s+\sqrt{\xi}+\sqrt{\xi_1}\right)H(\xi-\xi_1) + \{\Psi_\xi n^{\mathrm{ph}}_{\xi_1-\xi}\left(1+\Psi_{\xi_1}\right) - \left(1+\Psi_\xi\right)\left(1+n^{\mathrm{ph}}_{\xi_1-\xi}\right)\Psi_{\xi_1}\}\times H\left(Q_{as}+\sqrt{\xi}-\sqrt{\xi_1}\right)H\left(-Q_{as}+\sqrt{\xi}+\sqrt{\xi_1}\right)H\left(\sqrt{\xi_1}-\sqrt{\xi}\right)\}]$…… (11)

Where $\mathrm{C}_1 = \frac{D^2\sqrt{M_x}}{4\sqrt{2}\rho\pi\hbar^4 v_s^4}$ and $Q_{s/as} = \frac{\xi-\xi_1}{\sqrt{2M_x}v_s}$

For zero energy we get the equation

$$\left(\frac{\partial\Psi_{\xi=0}}{\partial t}\right)_{ex-ph} = \mathrm{C}_2\left[\Psi_{\xi_0}\left(1+n^{\mathrm{ph}}_{\xi_0}\right) - \Psi_{\xi=0}\left(n^{\mathrm{ph}}_{\xi_0}-\Psi_{\xi_0}\right)\right] \qquad \ldots\ldots\ldots\ldots\ldots\ldots (12)$$

With $\mathrm{C}_2 = \frac{4D^2{M_x}^3 v_s}{\rho\pi\hbar^4}$

3.2.1 Numerical Modelling

We discretize the energy $\xi = (l-1)\Delta\xi$ where $l = 1\ to\ n$ and $\Delta\xi = \frac{\xi_0}{m}$ with m is an integer. Similarly, we discretize the energy $\xi_1 = (q-1)\Delta\xi$. After discretization we can write the equation as

$$\left(\frac{\partial\Psi_l}{\partial t}\right)_{ex-ph} = -\frac{C_3}{m^{\frac{5}{2}}\sqrt{l-1}}\sum_{q_{min}}^{q_{max}}(l-q)^2 \times [\{\Psi_l(1+n_{l-q}^{ph})(1+\Psi_q)-(1+\Psi_l)n_{l-q}^{ph}\Psi_q\}$$

$$+\{\Psi_l n_{q-l}^{ph}(1+\Psi_q)-(1+\Psi_l)(1+n_{q-l}^{ph})\Psi_q\}] \quad \text{.......................} (13)$$

With $C_3 = \frac{D^2 {M_x}^3 v_s}{\rho\pi\hbar^4}$ and $n_{l-q}^{ph} = \frac{1}{\exp\left\{\frac{\xi_0(l-q)}{k_B T m}\right\}-1}$. Where, T is the lattice temperature. Then we can write the equation as below

$$\left(\frac{\partial\Psi_l}{\partial t}\right)_{ex-ph} = -\frac{C_3}{m^{\frac{5}{2}}\sqrt{l-1}}\sum_{q_{min}}^{q_{max}}(l-q)^2 \times [\{\Psi(j,l)(1+\frac{1}{\exp\left\{\frac{\xi_0(l-q)}{k_B T m}\right\}-1})(1+\Psi(j,q))-(1+\Psi(j,l))\frac{1}{\exp\left\{\frac{\xi_0(l-q)}{k_B T m}\right\}-1}\Psi(j,q)\}+\{\Psi(j,l)\frac{1}{\exp\left\{\frac{\xi_0(q-l)}{k_B T m}\right\}-1}\left(1+\Psi(j,q)\right)-\left(1+\Psi(j,l)\right)\left(\frac{1}{\exp\left\{\frac{\xi_0(q-l)}{k_B T m}\right\}-1}\right)\Psi(j,q)\}] \quad \text{..............}(14)$$

The values of q_{min} and q_{max} for Stokes and anti-Stokes scattering has been calculated from the Dirac Delta function of equation (9). For Stokes scattering q_{min} and q_{max} are $\left(\sqrt{l-1}-\sqrt{m}\right)^2$ and $l-1$ respectively. For anti-Stokes scattering q_{max} is $\left(\sqrt{l-1}-\sqrt{m}\right)^2$ and q_{min} is the maximum of $l-1$ and $\left(\sqrt{l-1}-\sqrt{m}\right)^2$.

For zero energy we can write the equation as below

$$\left(\frac{\partial\Psi_{l=1}}{\partial t}\right)_{ex-ph} = C_2\left[\Psi_{\xi_0}\left(1+n_{\xi_0}^{ph}\right)-\Psi_{l=1}\left(n_{\xi_0}^{ph}-\Psi_{\xi_0}\right)\right] \quad \text{........................} (15)$$

3.3 Radiative and non-radiative decay

The radiative and non-radiative decay equation is given below

$$\left(\frac{\partial \boldsymbol{\Psi}_{\vec{k}}}{\partial t}\right)_{R-nr-decay} = -\boldsymbol{\Upsilon}_p \boldsymbol{\Psi}(\vec{\boldsymbol{r}}, \boldsymbol{\xi}) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(16)}$$

Here Υ_p is decay rate. By numerical modelling we get

$$\left(\frac{\partial \Psi_l}{\partial t}\right)_{R-nr-decay} = -\Upsilon_p \Psi(j, l) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(17)}$$

3.4 Auger Decay

The details of Auger Decay have been discussed in the reference [16]. The equation of Auger Decay is given by

$$\left(\frac{\partial \Psi_{\vec{k}}}{\partial t}\right)_{AG-decay} = -\mathrm{C}_{AG} L_d(\vec{r}) \Psi(\vec{r}, \vec{k}) + \frac{1}{2} \mathrm{C}_{AG} \left(L_d(\vec{r})\right)^2 . \frac{(2\pi)^3}{\int d^3\vec{k}} \ldots\ldots\ldots\ldots\ldots\ldots \text{(18)}$$

Where $\int d^3\vec{k} = \int_0^{\xi_{max}} \frac{4\sqrt{2}\pi M_x^{3/2}}{\hbar^3} \sqrt{\xi}\, d\xi$ and

$$L_d(\vec{r}) = \frac{1}{(2\pi)^3} \int 4\pi k^2\ \Psi(\vec{r}, \vec{k}) dk = \frac{1}{(2\pi)^3} \int \frac{4\sqrt{2}\pi M_x^{3/2}}{\hbar^3} \Psi(\vec{r}, \xi) \sqrt{\xi}\, d\xi \ldots\ldots\ldots\ldots \text{(19)}$$

3.4.1 Numerical Modelling

We discretize the energy $\xi = (l-1)\Delta\xi$ where $l = 1\ to\ n$ and $\Delta\xi = \frac{\xi_0}{m}$ with m is an integer. After discretization we can write the equation as

$$L_d(l) = L_d(\vec{r}) = \frac{1}{(2\pi)^3} \sum \frac{4\sqrt{2}\pi M_x^{\frac{3}{2}} {\xi_0}^{\frac{3}{2}}}{\hbar^3 m^{\frac{3}{2}}} \sqrt{l-1}\, \Psi(j, l)$$

$$= \frac{1}{(2\pi)^3} \sum_{l=0}^{l=l_{max}} \frac{\mathrm{C}_4}{m^{3/2}} \sqrt{l-1}\, \Psi(j, l) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(20)}$$

Where $\mathrm{C}_4 = \frac{4\sqrt{2}\pi M_x^{3/2}{\xi_0}^{3/2}}{\hbar^3}$

$I_l = \int d^3\vec{k} = \sum_{l=0}^{l=l_{max}} \frac{4\sqrt{2}\pi M_x^{3/2}{\xi_0}^{3/2}}{\hbar^3 m^{3/2}}\sqrt{l-1} = \sum_{l=0}^{l=l_{max}} \frac{\mathrm{C}_4}{m^{3/2}}\sqrt{l-1}$ ..... (21)

$\left(\frac{\partial \Psi_l}{\partial t}\right)_{AG-decay} = -\mathrm{C}_{AG} L_d(l)\, \Psi(j,l) + \frac{1}{2}\mathrm{C}_{AG}\left(L_d(\vec{r})\right)^2 . \frac{(2\pi)^3}{I_l}$ ..... (22)

3.5 Exciton-Exciton Collision

Two body collision of the Boson gas can be represented by Exciton-exciton collision term of the Boltzmann equation. In this case excitons of momenta $\vec{p}$ and $\vec{p}_1$ scatter into $\vec{k}$ and$\overrightarrow{k_1}$. All events of the exciton collision in and out of the volume $\left(d^3\vec{k}\right)$ of k space are involved in this equation. The net collision rate is given by

$$\left(\frac{\partial \Psi_{\vec{k}}}{\partial t}\right)_{ex-ex} d^3\vec{k} = \frac{2\pi}{\hbar}\cdot\frac{V^2}{(2\pi)^6}\int d^3\vec{k} d^3\vec{p}\, d^3\vec{p}_1 d^3\vec{k}_1 M^2_{matrix}$$

$\times [\{\Psi_{\vec{p}}\Psi_{\vec{p}_1}(1+\Psi_{\vec{k}})(1+\Psi_{\vec{k}_1})\} \times \delta(\vec{p}+\vec{p}_1-\vec{k}-\vec{k}_1)\delta(\xi_{\vec{p}}+\xi_{\vec{p}_1}-\xi_{\vec{k}}-\xi_{\vec{k}_1}) -$
$\{\Psi_{\vec{k}}\Psi_{\vec{k}_1}(1+\Psi_{\vec{p}})(1+\Psi_{\vec{p}_1})\} \times \delta(\vec{k}+\vec{k}_1-\vec{p}-\vec{p}_1) \times \delta(\xi_{\vec{k}}+\xi_{\vec{k}_1}-\xi_{\vec{p}}-\xi_{\vec{p}_1})]$..... (23)

The collision rate of the excitons into state $\overrightarrow{k}$ is represented by the first part of the equation and the collision rate out of state$\vec{k}$ is represented by the second part of the equation.$\Psi_{\vec{k}}$,$\Psi_{\vec{p}}$, $\Psi_{\vec{p}_1}$and $\Psi_{\vec{k}_1}$ are the excitons occupation number in $\vec{k}$ state, $\vec{p}$ state, $\vec{p}_1$state, and $\vec{k}_1$ state, respectively. Here$\xi_{\vec{k}} = \hbar^2k^2/2M_x$, $\xi_{\vec{p}} = \hbar^2p^2/2M_x$, $\xi_{\vec{p}_1} = \hbar^2{p_1}^2/2M_x$ and $\xi_{\vec{k}_1} = \hbar^2{k_1}^2/2M_x$ are the excitons energy in wave vector $\vec{k}$ state, $\vec{p}$ state, $\vec{p}_1$ state, and $\vec{k}_1$ state,

respectively. $M_{matrix} = \frac{4\pi\hbar^2 a_1}{M_x \mathrm{V}}$ is the matrix element [14] and a_1 is the scattering length.$\xi_{\vec{k}_1} = \xi_{\vec{p}} + \xi_{\vec{p}_1} - \xi_{\vec{k}}andk_1 = \sqrt{\vec{p}^2 + \vec{p}_1^2 - \vec{k}^2}$. In this case $\vec{k}_1$ is one out scattering momentum, $\vec{p}$ and $\vec{p}_1$are two in scattering momenta of excitons.

Then to solve numerically all momentum $(\vec{k})$ terms of the equation (23) has been transferred to energy terms $(\vec{\xi})$ terms by using equation (5). After that we get the four parts of the equation where the first part is for $\xi_{\vec{k}} > \xi_{\vec{p}}$ and $\xi_{\vec{k}} < \xi_{\vec{p}}$. The second part is for ground state mode for energy equal to zero$(\vec{k} = 0)$. The third part is for out scattering term equal to zero $(\vec{k}_1 = 0)$. The fourth part is for two in scattering terms equal to zero $\vec{p} = 0\ and\ \vec{p}_1 = 0$. The details have been given in the reference [17]. Exciton-exciton collision in homogeneous system have been studied by the researchers of reference [18].Therefore, we get the equation for exciton-exciton collision is given by

$$\left(\frac{\partial \Psi_{\xi_{\vec{k}}}}{\partial t}\right)_{ex_ex_whole} = \left(\frac{\partial \Psi_{\xi_{\vec{k}}}}{\partial t}\right)_{ex_ex} + \left(\frac{\partial \Psi_{\xi_{\vec{k}}=0}}{\partial t}\right)_{zero_energy} + \left(\frac{\partial \Psi_{\xi_{\vec{k}_1}=0}}{\partial t}\right)_{out_scatt_zero} + 2 \cdot \left(\frac{\partial \Psi_{\xi_{\vec{p}_1}=0}}{\partial t}\right)_{in_scatt_zero} \quad \text{..... (24)}$$

3.5.1 Numerical Modelling

To do the numerical modelling, the energy $\xi_{\vec{k}}$ has been discretized by $\xi_{\vec{k}} = \left(l_{\vec{k}} - 1\right)\Delta\boldsymbol{\xi}$ where$l_{\vec{k}} = 1\ldots\ldots n$, n is an integer and $\Delta\xi = \frac{\xi_0}{m}$ with M is an integer. Analogously, other energies have been discretized by$\xi_{\vec{k}_2} = \left(l_{\vec{k}_2} - 1\right)\Delta\boldsymbol{\xi}$, $\xi_{\vec{p}} = (l_{\vec{p}} - 1)\Delta\boldsymbol{\xi}$ and $\xi_{\vec{p}_2} = (l_{\vec{p}_2} - 1)\Delta\boldsymbol{\xi}$. After discretization we get

$$\left(\frac{\partial \Psi_{\xi_{\vec{k}}}}{\partial t}\right)_{ex_ex} = \left(\frac{\partial \Psi_{l_{\vec{k}}}}{\partial t}\right)_{ex_ex} = \frac{4a_1^2 M_x}{\pi \hbar^3} \cdot \frac{1}{\sqrt{l_{\vec{k}}-1}} \cdot \left(\frac{\xi_0}{m}\right)^2$$

$$\times \left[\sum_{0}^{l_{\vec{k}}} \sum_{l_{\vec{k}}-l_{\vec{p}}}^{\infty} \min[\sqrt{l_{\vec{p}}-1}, \sqrt{l_{\vec{p}_1}-1}, \sqrt{l_{\vec{k}}-1}, \sqrt{l_{\vec{k}_1}-1}] \right.$$

$$\left. + \sum_{l_{\vec{k}}}^{\infty} \sum_{0}^{\infty} \min[\sqrt{l_{\vec{p}}-1}, \sqrt{l_{\vec{p}_1}-1}, \sqrt{l_{\vec{k}}-1}, \sqrt{l_{\vec{k}_1}-1}] \right]$$

$$\times [\{\Psi_{l_{\vec{p}}} \Psi_{l_{\vec{p}_1}} (1+\Psi_{l_{\vec{k}}})(1+\Psi_{l_{\vec{k}_1}})\}$$

$$-\{\Psi_{l_{\vec{k}}} \Psi_{l_{\vec{k}_1}} (1+\Psi_{l_{\vec{p}}})(1+\Psi_{l_{\vec{p}_1}})\}] \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (25)$$

Or,

$$\left(\frac{\partial \Psi_{l_k}}{\partial t}\right)_{ex_ex} = \frac{4a_1^2 M_x}{\pi \hbar^3} \cdot \frac{1}{\sqrt{l_{\vec{k}}-1}} \cdot \left(\frac{\xi_0}{m}\right)^2 \times$$
$$\left[\sum_0^{l_{\vec{k}}} \sum_{l_{\vec{k}}-l_{\vec{p}}}^{\infty} \min[\sqrt{l_{\vec{p}}-1}, \sqrt{l_{\vec{p}_1}-1}, \sqrt{l_{\vec{k}}-1}, \sqrt{l_{\vec{k}_1}-1}] + \right.$$
$$\left. \sum_{l_{\vec{k}}}^{\infty} \sum_0^{\infty} \min\left[\sqrt{l_{\vec{p}}-1}, \sqrt{l_{\vec{p}_1}-1}, \sqrt{l_{\vec{k}}-1}, \sqrt{l_{\vec{k}_1}-1}\right]\right] \times [\{\Psi(j,l_p)\Psi(j,l_{p_1})(1+\Psi(j,l_k))(1+$$
$$\Psi(j,l_{k_1}))\} - \{\Psi(j,l_k)\Psi(j,l_{k_1})(1+\Psi(j,l_p))(1+\Psi(j,l_{p_1}))\}] \ldots\ldots\ldots\ldots\ldots\ldots\ldots (26)$$

The equation for zero energy state $(\vec{k}=0)$ i.e., when $l_{\vec{k}} = 1$, the equation will be

$$\left(\frac{\partial \Psi_{l_k=1}}{\partial t}\right)_{zero_energy} = \frac{4a_1^2 M_x}{\pi \hbar^3} \cdot \left(\frac{\xi_0}{m}\right)^2 \times \left[\sum_0^{\infty} \sum_0^{\infty} [\{\Psi_{l_{\vec{p}}} \Psi_{l_{\vec{p}_1}} (1+\Psi_{l_{\vec{k}}=1})(1+\Psi_{l_{\vec{k}_1}})\} - \right.$$
$$\left. \{\Psi_{l_{\vec{k}}=1} \Psi_{l_{\vec{k}_1}} (1+\Psi_{l_{\vec{p}}})(1+\Psi_{l_{\vec{p}_1}})\}]\right] \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (27)$$

Or,

$$\left(\frac{\partial \Psi_{l_{\vec{k}}=1}}{\partial t}\right)_{zero_energy} = \frac{4a_1^2 M_x}{\pi\hbar^3} \cdot \left(\frac{\xi_0}{m}\right)^2 \times \left[\sum_0^\infty \sum_0^\infty [\{\Psi(j,l_p)\Psi(j,l_{p_1})(1+\Psi(j,1))(1+\Psi(j,l_{k_1}))\} - \{\Psi(j,1)\Psi(j,l_{k_1})(1+\Psi(j,l_p))(1+\Psi(j,l_{p_1}))\}\right] \ldots\ldots\ldots\ldots\ldots\ldots (28)$$

The equation for out scattering term $\vec{k}_1$ equal to zero i.e., when $l_{\vec{k}_1} = 1$, the equation will be

$$\left(\frac{\partial \Psi_{\xi_{\vec{k}_1}=0}}{\partial t}\right)_{out_scatt_zero} = \left(\frac{\partial \Psi_{l_{\vec{k}_1}=1}}{\partial t}\right)_{out_scatt_zero} = \frac{4a_1^2}{\pi\sqrt{2M_x}} \cdot \frac{\Psi_{l_{\vec{k}_1}=1}}{V} \times \left(\frac{\xi_0}{m}\right)^{1/2} \times \sum_{l_{\vec{p}}=0}^{k} \frac{1}{\sqrt{l_{\vec{k}}-1}} \cdot \{\Psi_{l_{\vec{p}}}\Psi_{l_{\vec{p}_1}} - \Psi_{l_{\vec{k}}}(1+\Psi_{l_{\vec{p}_1}} + \Psi_{l_{\vec{p}}})\}$$

…… (29)

Or,

$$\left(\frac{\partial \Psi_{l_{\vec{k}_1}=1}}{\partial t}\right)_{out_{scatt_{zero}}} = \frac{4a_1^2}{\pi\sqrt{2M_x}} \cdot \frac{\Psi(j,1)}{V} \times \left(\frac{\xi_0}{m}\right)^{\frac{1}{2}} \times \sum_{l_{\vec{p}}=0}^{k} \frac{1}{\sqrt{l_{\vec{k}}-1}} \cdot \{\Psi(j,l_p)\Psi(j,l_{p_1}) - \Psi(j,l_k)(1+\Psi(j,l_{p_1})+\Psi(j,l_p))\}$$ …… (30)

The equation for in scattering term $\vec{p}_1$ equal to zero i.e., when $l_{\vec{p}_1} = 1$ the equations can be written in the form of

$$\left(\frac{\partial \Psi_{\xi_{\vec{p}_1}=0}}{\partial t}\right)_{in_scatt_zero} = \left(\frac{\partial \Psi_{l_{\vec{p}_1}=1}}{\partial t}\right)_{in_scatt_zero} = \frac{4a_1^2}{\pi\sqrt{2M_x}} \cdot \frac{\Psi_{l_{\vec{p}_1}=1}}{V} \cdot \left(\frac{\xi_0}{m}\right)^{1/2} \times \sum_{l_{\vec{p}}=k}^{\infty} \frac{1}{\sqrt{l_{\vec{k}}-1}} \cdot \{\Psi_{l_{\vec{p}}}(1+\Psi_{l_{\vec{k}_1}}+\Psi_{l_{\vec{k}}}) - \Psi_{l_{\vec{k}}}\Psi_{l_{\vec{k}_1}}\} \ldots\ldots\ldots\ldots\ldots\ldots (31)$$

Or,

$$\left(\frac{\partial \Psi_{l_{\vec{p}_1}=1}}{\partial t}\right)_{in_scatt_zero} = \frac{4a_1^2}{\pi\sqrt{2M_x}} \cdot \frac{\Psi(j,1)}{V} \cdot \left(\frac{\xi_0}{m}\right)^{1/2}$$

$$\times \sum_{l_{\vec{p}}=k}^{\infty} \frac{1}{\sqrt{l_{\vec{k}}-1}} \cdot \{\Psi(j,l_p)(1+\Psi(j,l_{k_1})+\Psi(j,l_k)) - \Psi(j,l_k)\Psi(j,l_{k_1})\} \ldots\ldots\ldots\ldots \quad (32)$$

3.6 Initial and Boundary Conditions

In this calculation laser excitation has been used. The laser beam at energy ξ_L crosses the trap centrally with respect to the bottom energy of the trap and create excitons at $\xi = \xi_L - c\vec{r}^2$. Therefore, the initial distribution can be written as

$$\Psi_{initial}(\vec{r},\xi) = \mathrm{C}_0\, exp\left(\frac{-(\xi-(\xi_L-c\vec{r}^2))^2}{2\beta^2}\right) \times H(\vec{r}_{max}-\vec{r})H(\vec{r}) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (33)$$

Here, C_0 represents the overall number of excitons, β represents the spectral width and $r_{max} = \sqrt{2\xi_L/\beta}$ represents the maximum radius.

The boundary conditions are fixed in such a way that no exciton flows take place outside the trap. These are

(i) The rate of change of exciton number with respect to radius is zero $\left(\frac{\partial \Psi}{\partial r} = 0\right)$ at $r < 0$ and at $r > r_{max}$ for all values of energy.

(ii) The rate of change of exciton number with respect to radius is zero $\left(\frac{\partial \Psi}{\partial r} = 0\right)$ at $\xi > \xi_{max}$ for all values of radius.

(iii) The rate of change of exciton number with respect to energy is zero $\left(\frac{\partial \Psi}{\partial \xi} = 0\right)$ at $\xi < 0$ and at $\xi > \xi_{max}$ for all values of radius.

(iv) The rate of change of exciton number with respect to energy is zero $\left(\frac{\partial \Psi}{\partial \xi} = 0\right)$ at $r > r_{max}$ for all values of energy.

4. Description of the program

There are two .m files for running the program written by MATLAB code. One is programme_source.m file and another is programme_main.m file. In the source file the program has been written for the calculation of drift term, force term, exciton-phohnon collision, exciton-exciton collision, Auger decay, Radiative and non-radiative decay (see equation (3)). Boundary conditions also have been included in the source file. In the

programme_main.m file the value of different parameters has been given. Grid for energy and momentum direction has been set up. Initial condition and the time limit for the integration has been given. Then ode15s function has been used for integration over time to get exciton occupation number over time (see equation (3)). Source file has been called through ode15s function to do the integration. Then 1D matrix has been converted into 2D matrix and as a result exciton occupation number is obtained as a function of time, radius and momentum.

4.1 About Programme_main.m file:

4.1.1 Global

First, we call some parameters as global parameters as given below. Therefore, if we put the values of the parameters in programme_main.m file it will be used by another file programme_source.m. We do not need to put the values in both files.

```
% Global area
global nr  ne  dr de r e  Nel rl N0 c  M c1 c2 c6  ncall
```

4.1.2 Values of parameters

Then we have set the values of different parameters which have been used in this program (see below). If we have to change the values of the parameters then we can change it here.

```
% Model parameters

el=100;
rl=200;

Mx=2.61*9.109*10^(-31);  %kg
M=95;
v=4500; %m/s
h1=1.055*10^(-34);  %Joul.second
c3=(4*(Mx^2)*(v^2))/((h1^2)*(M));
e0=601.04;          %micro_ev
a=0.801*10^(-25);  % unit Joul/micro_m^2
kB=1.381*10^(-23);  % unit J/k
alp=(0.5*M)/(e0);

c1=(9)/(sqrt(M));      [unit=micro_m/ns]
c2=0.01497*(sqrt(M)); [unit=1/(micro_m*ns)]
c4=(1/((2*pi)^3))*((((4*pi)^2)*sqrt(2)*(Mx^(3/2)))/(h1^3))*(((e0*1.602*10^(-
25))/M)^(3/2))*(10^(-18));
```

```
h=6.972;            %h=e0/K_B=(2*Mx*v^2)/k_B  [unit=kelvin]
tem=0.1;
c=(h/(tem*M));
n0=6*10^(-2);
c6=95.275;
```

4.1.3 Grid setting

The grid in the momentum direction (k) and radius direction (r) has been set in the following way

```
% Grid in k direction
  ne=100;
  de=el/(ne-1);

  for j=1:ne
    e(j)=(j-1)*de;
  end
%
% Grid in r direction
  nr=100;
  dr=rl/(nr-1);

  for i=1:nr
    r(i)=(i-1)*dr;
  end
```

4.1.4 Setting independent variable for integration

In this case time is independent variable. Time limit has been set from 0 to 200 ns. Interval is 1. Therefore, there are 201 points between 0 to 200 ns.

```
Independent variable (time) for ODE integration
tf=200;
  tout=(0:1:tf)';
nout=201;
ncall=0;
```

4.1.5 Pre allocation of space

We have pre allocate the space to get speed in the program in the following way

```
% Preallocation for speed
N0=zeros(nr,ne);
y0=zeros(nr,ne);
N_rad_1=zeros(nr,ne);
N_rad_5=zeros(nr,ne);
N_rad_10=zeros(nr,ne);
```

4.1.6 Initial condition

Initial condition for the integration has been set in the following way. In this case it is gaussian distribution.

```
% Initial condition
  for i=1:nr
  for j=1:ne
     if (i>=35)
        N0(i,j)=0;
     else
        N0(i,j)=n0*(exp((-(j-(45-(alp.*((r(i)).^2)))).^2)/(2*(3)^2)));

     end

        y0((i-1)*ne+j)=N0(i,j);

  end
  end
```

4.1.7 Integrationof the differential equation

Here ode15s has been used to do integration. This function calls "mypde_with_s_PS_ES_condensate_term_RR_TBD" from the programme_source.m file and does the calculation for the given parameters.

```
%ODE integration

[t,y]=ode15s(@programme_source,tout,y0);
```

4.1.8 Conversion of one dimensional to two-dimensional matrix

After doing the integration we get the value of y as a function of time(t) and another variable, which is an array that mixed of both radius and momentum vector. Then to get y as a function of time(t), radius (r) and momentum (k) we transfer 1D array to 2D matrix in the following way.

```
%   1D to 2D matrices
  for it=1:nout
  for i=1:nr
  for j=1:ne
    N(it,i,j)=y(it,(i-1)*ne+j);
    N(1,i,j)=y0((i-1)*ne+j);
    N(1,i,j)=N0(i,j);

  end
  end
  end
```

4.1.9 Radial profile

Using the following way we have calculated the exciton distribution for a particular time. Below programming is for 5ns.

```
% Radial profiles (at t = tf)
for i=1:nr
  for j=1:ne
    N_rad_5(i,j)=N(5,i,j);
  end
  end
```

4.2 About Programme_source.m file:

4.2.1 Setting function

The programme_source.m file has been set as function (see below) with name yt and it will be called by ODE integrator, ode15s in the programme_main.m file.

```
function yt= programme_source(~,y)
```

4.2.2 Global

We set some parameters as global parameters as it has been described in the section 3.1.1, (see below).

```
% Global area
global nr  ne  dr N  M c1  c2 c6  c ncall
```

4.2.3 Conversion of one dimensional to two-dimensional matrix

To do the calculation we convert one dimensional to two-dimensional matrices in the following way

```
% 1D to 2D matrices
  for i=1:nr
  for j=1:ne
ij=(i-1)*ne+j;
    N(i,j)=y(ij);

  end
  end
```

4.2.4 Pre allocation of space

As we discussed in the section 3.1.5 in the same way we have pre allocate the space to get speed in the program in the following way

```
% Preallocation for speed
frd=zeros(nr,ne);
ftbd=zeros(nr,ne);
  N1=zeros(nr,ne);
  N2=zeros(nr,ne);
  f=zeros(nr,ne);
```

4.2.5 Programming for exciton-phonon collision, exciton-exciton collision, Auger decay and radiative non-radiative decay

```
% exciton phonon collision
% exciton exciton collision
% radiative and non-radiative decay
% Auger decay
```

In this part we have given programming code for the exciton phonon collision, radiative non-radiative decay, Auger decay and exciton-exciton collision.We have discussed about these collisions process in the section 2.2, 2.3, 2.4 and 2.5 respectively.

4.2.6 Boundary conditions

We have set boundary condition in this way that no exciton flows take place outside of the trap. It has been discussed in the section 2.5. In the programming of the boundary conditions (see below) Nt(i,j) represents $\frac{\partial \Psi}{\partial t}$ of the equation (3).

```
% Boundary condition
  for i=1:nr
  for j=1:ne


     if(i==1)
        Nr(i,j)=0;
     elseif(i==nr)
        Nr(i,j)=0;
     elseif(j==ne)
        Nr(i,j)=0;
     else
         Nr(i,j)=((N(i,j)-N(i-1,j))/dr);
    end

     if(j==ne)
         Ne(i,j)=0;
     elseif(j==1)
         Ne(i,j)=0;
     elseif(i==nr)
         Ne(i,j)=0;
     else
         Ne(i,j)=((N(i,j+1)-N(i,j)));
End

Nt(i,j)=-(c1*sqrt(j).*Nr(i,j))+(c2*sqrt(j).*(i-1).*dr.*Ne(i,j))+f(i,j)+fes(i,j)-frd(i,j)+ftbd(i,j);


  end
  end
```

4.2.7 Two dimensional to one dimensional matrix

```
% 2D to 1D matrices
  for i=1:nr
  for j=1:ne
ij=(i-1)*ne+j;
yt(ij)=Nt(i,j);
  end
  end
```

In this part we transfer two dimensional to one dimensional matrix to integrate it by ode15s function.

5. How to use BTELAB

To do the calculation, MATLAB software should be installed in the computer. Then programme_source.m and programme_main.m files should be saved in C directory of the computer. After setting the values of different parameters and the limit of integration in the programme_main.m file we have to press run in the programme_main.m file to run the program. Programme_main.m file automatically called the function in the programme_source.m file through ode15s function. By writing the code for save in the programme_main.m file result will be saved in the mentioned directory as a .mat file.

6. Results

6.1Numerical Stability

Numerical stability is an important issue in the case of numerical simulation. In this case, it has been checked by possible loss or gain of excitons with time within a finite region or space. If there is no such possible loss or gain of excitons with time then we can say that our numerical simulation has numerical stability. To check it, a series of simulations with different initial exciton number have been done for T=0.1 K. Then total number of excitons has been plotted over time for each initial exciton number (Fig. 1). The total number of excitons has been calculated by the equation

$$\Psi_{total} = \frac{1}{(2\pi)^3} \int_0^\infty \int_0^\infty 4\pi r^2 dr . 4\pi k^2 dk . \Psi(r,k)$$

Figure 1 shows that the total number of excitons (N_{total}) versus time curves for 0.1 K with the volume of 1 mm^3. Here it has been seen that with low initial number of excitons and high initial number of excitons for both cases in the beginning and at the 100 ns, the total number of excitons is almost same but from 10 ns to 50 ns it is slightly decreasing and then again increasing.

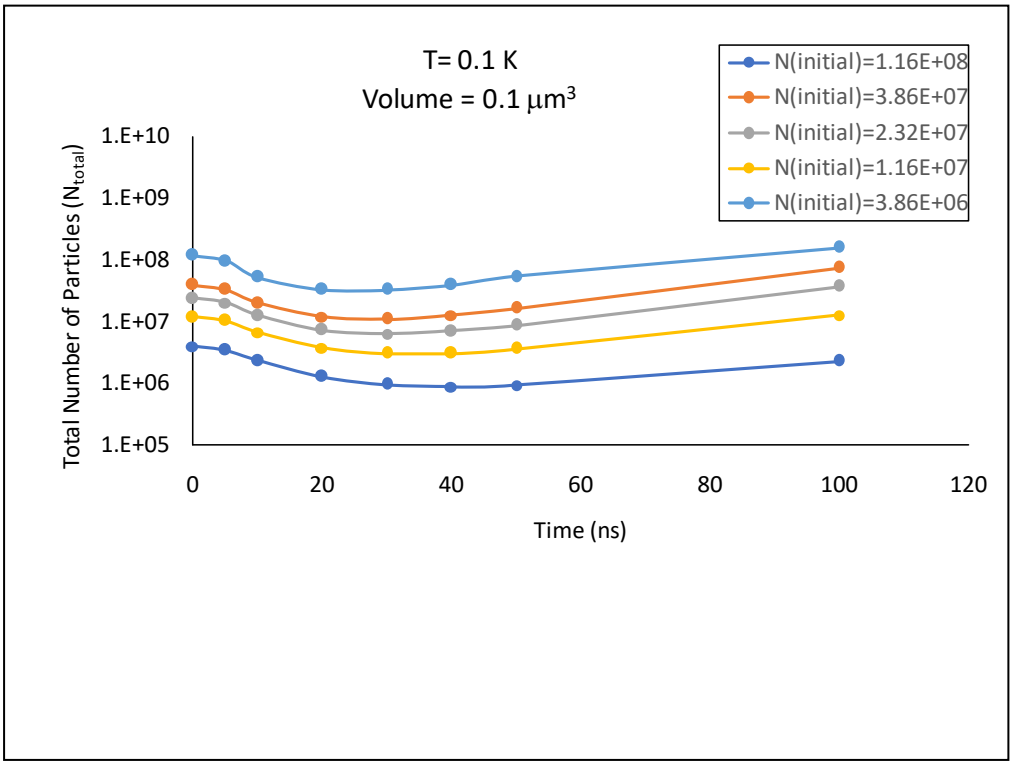


Fig 1: Total number of excitons versus time for 0.1 K with the volume of 1 mm^3 including exciton-phonon collision, exciton-exciton collision, Auger decay, radiative and non-radiative decay. The curves show that how the total number of excitons is changing with time for different initial exciton number.

6.2 High number of excitons

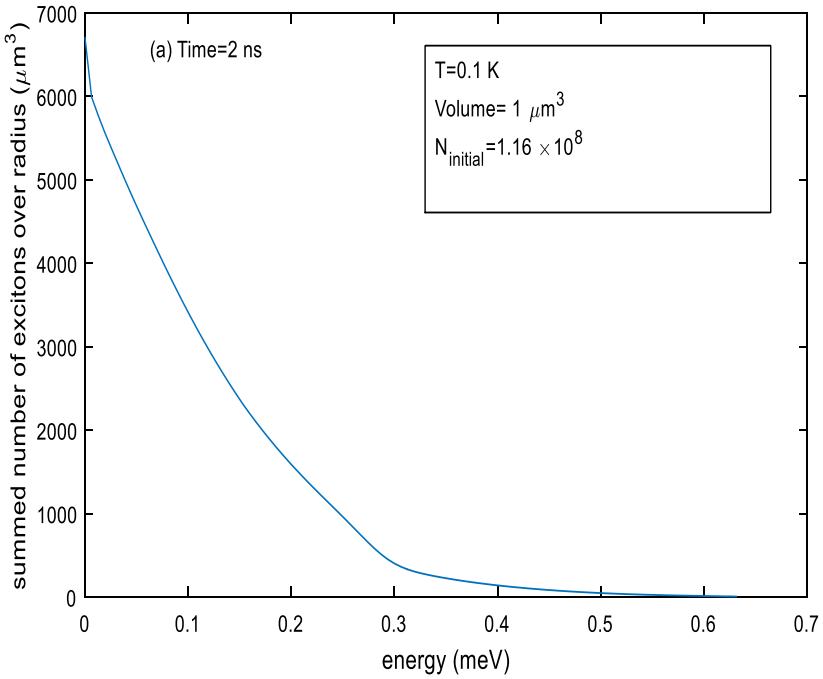
From the previous research work, it has been seen that the BEC can be obtained for sufficiently high number of excitons, when the exciton number is above the critical number of excitons. To check the numerical program is working properly or not, few numerical simulations have been done for the exciton number over the critical number of excitons. This behaviour is observed clearly in the exciton occupation (n_r) vs. energy curves. The exciton occupation (n_r) has been calculated by summed number of excitons over the radius. The mathematical formulation of (n_r) is given by

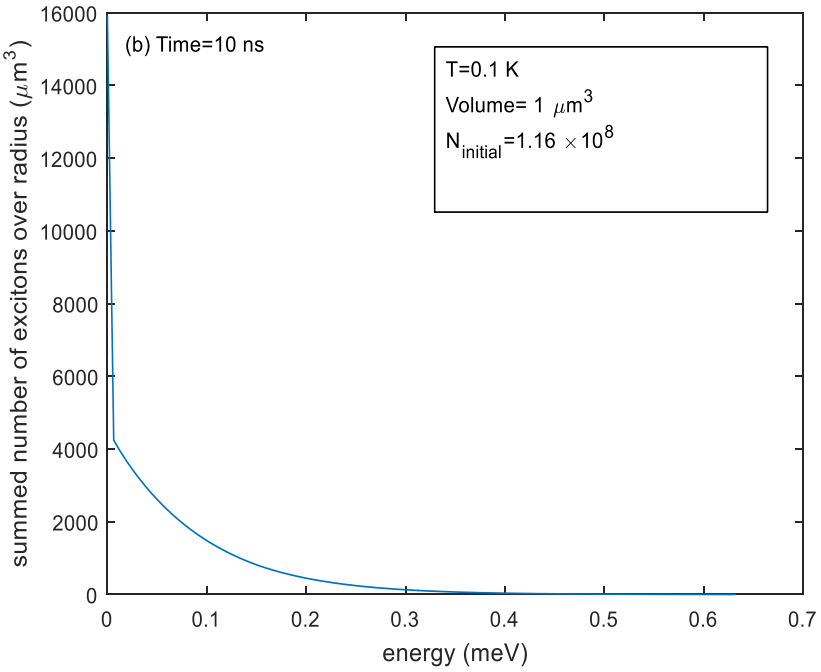
$$n_r(\xi) = \int_0^{\infty} N(r,\xi).\,4\pi r^2 dr$$

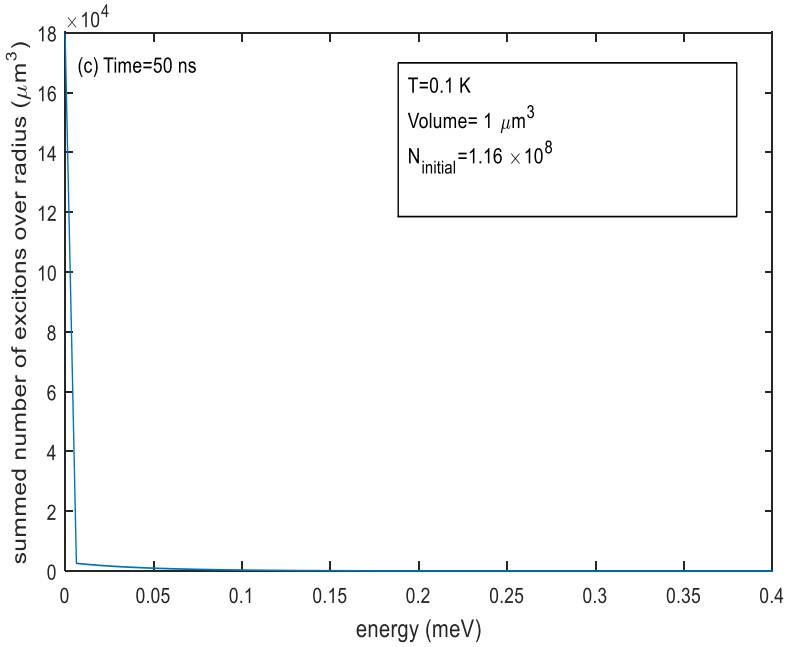
Figure 2 shows exciton occupation n_r vs. energy curves at 0.1 K for different times with the initial total numbers of excitons are 1.16×10^8 and volume is 1 mm^3.The critical number of excitons for 0.1 K is 1.53×10^5.The critical number of excitons $\boldsymbol{N_c}$ has been calculated by the equation below.

$$N_c = 1.202\left(\frac{K_B T}{\hbar\sqrt{\frac{2\alpha}{M_x}}}\right)$$

Therefore, here the initial total number of excitons is greater than the critical number of excitons for 0.1 K. Figure 2 shows how exciton occupation distribution is changing with time. At 2 ns (Fig. 2(a)) exciton occupation takes Boltzmann distribution, at 10 ns (Fig. 2(b)) it takes Bose-Einstein distribution, at 50 ns (Fig. 2(c)) the distribution is coming very close to zero energy and at 100 ns a high peak near zero energy indicates the BEC is formed and it is stable over long time. From these results it can be said that our program is working properly.


(a) Time=2 ns
T=0.1 K
Volume= 1 μm3
Ninitial=1.16 ×108
summed number of excitons over radius (μm3)
energy (meV)
0
1000
2000
3000
4000
5000
6000
7000
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7


(b) Time=10 ns
T=0.1 K
Volume= 1 μm^3
N$_{initial}$=1.16 $\times$10^8
summed number of excitons over radius (μm^3)
energy (meV)
16000
14000
12000
10000
8000
6000
4000
2000
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7


×10^4
18
16
14
12
10
8
6
4
2
0
summed number of excitons over radius (μm^3)
(c) Time=50 ns
T=0.1 K
Volume= 1 μm^3
N_initial=1.16 ×10^8
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
energy (meV)

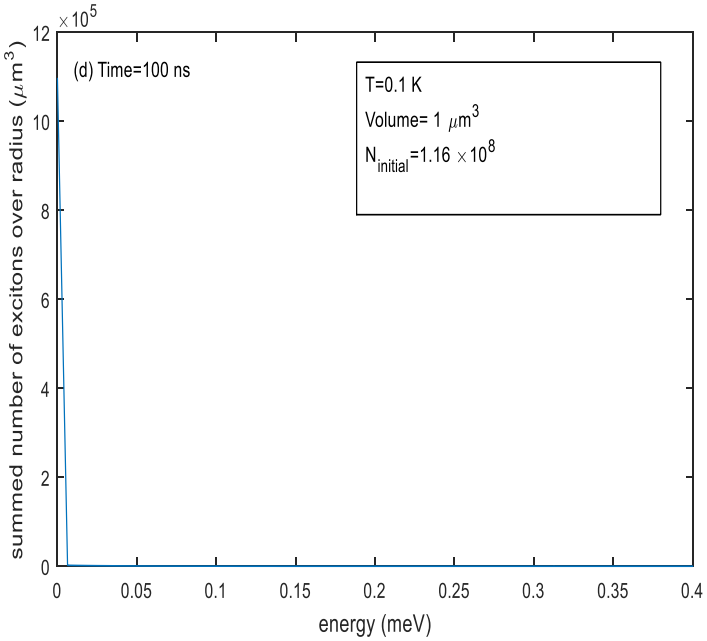


Figure 2: Exciton occupation distribution by summed number of excitons over radius versus energy curves in linear scale at 0.1 K for different times. The initial total numbers of excitons are 1.16×10^8 and volume is 1 mm^3. (a), (b), (c), and (d) show exciton occupation at 2 ns, 10 ns, 50ns and 100 ns respectively. Figures show how exciton distribution is coming close to zero energy and at 100 ns a high peak near zero energy indicates BEC.

7. Conclusions

In this paper we present BTELab which is a MATLAB toolbox for the computation of full Boltzmann Transport equation with all collision terms. Here it has been used to see the relaxation kinetics and Bose-Einstein condensation of excitons but it can be used to solve different other problem related to BEC. From the results it can be said that the program has enough numerical stability to get reliable results.

CRediT authorship contribution statement

Sunipa Som: Writing – original draft, Software, Methodology, Conceptualization; **Ravindra Dhar:** Writing – review & editing, Supervision; **Ram Kripal**: Writing – review & editing, Software, Supervision; **Heinrich Stolz**: Writing – review & editing, Software, Methodology, Conceptualization, Supervision

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Data availability

Data will be made available on request.

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Data availability

The datasets generated during and/or analysed during the current study are available from the corresponding author on reasonable request.

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