Globally hyperbolic moment method for BTE including phonon scattering

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***Abstract*— A globally hyperbolic high-order moment method of the Boltzmann transport equation (BTE) is proposed in [1], [2], and here it is extended for the BTE with the electron-phonon scattering term to simulate a silicon nano-wire (SNW). Convergence with respect to the order of the moment system and the characteristics of SNW including the I-V curve are studied.**

I. Introduction

The drift-diffusion (DD) derived from the BTE was the most popular tool in semiconductor simulation for a long time. As devices are scaling down to submicrometer, it fails in capturing the nonlocal and hot carrier effects. To overcome the limitation of the DD model, many high-order transport models are derived by closing the moment system via an Ansatz of the form of the distribution function. However, those closure relations are highly dependent on the model, so unfortunately, these closed moment methods have performed failure in different degrees [3]. Recently, a globally hyperbolic regularization is proposed in [1], [2]. Its most appealing feature is that the closure is done by fulfilling the hyperbolicity of the regularized moment system instead of a guess of Ansatz of the distribution function. Furthermore, the characteristic speeds of the regularized moment system can be analytically given and only depend on the macroscopic velocity and the temperature. The regularized moment system up to any order can be obtained systematically by the globally hyperbolic closure without calibrating any parameter. Additionally, it has been successfully developed in [4], [5] to validate the robustness of this method in simulating microflows, etc. In this paper, this method is applied to simulate a n^+-n-n^+ silicon nano-wire modeled by the electron-phonon scattering involved BTE. The convergence of the macroscopic quantities with respect to the order of the moment system can be observed obviously and some I-V curves are simulated at some orders.

II. Methodology

Electron transportation in a SNW is simulated with the semiclassical BTE

$$\frac{\partial f}{\partial t} + \frac{v}{m}\frac{\partial f}{\partial x} - V'(x)\frac{\partial f}{\partial v} = \frac{\partial f}{\partial t}|_{scat}, \tag{1}$$

where the potential energy $V(x)$ is calculated by the Poisson equation(PE). Both the acoustical-phonon scattering and the optical-phonon scattering are included. Following the method proposed in [6], [7], we expand the distribution function $f(t,x,v)$ into a M-order truncated series of the Hermite functions. The Hermite function $\mathcal{H}_\alpha(u(t,x),\mathcal{T}(t,x))$ for $\alpha = 0,1,\cdots,M$ defined as

$$\mathcal{H}_{\mathcal{T},\alpha}(\xi) = \frac{1}{\sqrt{2\pi}}\mathcal{T}^{-\frac{\alpha+1}{2}}H_\alpha(\xi)\exp\left(-\frac{\xi^2}{2}\right) \tag{2}$$

by using the Hermite polynomial

$$H_\alpha(\xi) = (-1)^\alpha \exp\left(\frac{\xi^2}{2}\right)\frac{\mathrm{d}^n}{\mathrm{d}\xi^n}\exp\left(-\frac{\xi^2}{2}\right) \tag{3}$$

is used as the basis function of the M-term expansion approximating $f(t,x,v)$ in the form of

$$f(t,x,v) \approx \sum_{\alpha=0}^{M} f_\alpha(t,x)\mathcal{H}_\alpha\left(\frac{v-u(t,x)}{\sqrt{\mathcal{T}(t,x)}}\right). \tag{4}$$

It is noted that the expansion (4) takes the mean velocity $u(t,x)$ as the shifting and the local scaled temperature $\mathcal{T}(t,x)$ as the scaling, with the expansion coefficients $f_\alpha, \alpha = 0,\cdots,M$.

As proposed in [1], a 1-D hyperbolically regularized quasi-linear moment system is obtained by substituting $\partial f_{M+1}/\partial x$ in the last moment equation of the corresponding M-th moment system with the linear combination of f_{M-1} and f_M, which is given as

$$\frac{\partial f_{M+1}}{\partial x} = -f_M\frac{\partial u}{\partial x} - \frac{1}{2}f_{M-1}\frac{\partial \mathcal{T}}{\partial x}. \tag{5}$$

The regularized quasi-linear moment system for collisionless BTE truncated up to M reads

$$\begin{aligned}&\frac{\partial f_\alpha}{\partial t} + \mathcal{T}\frac{\partial f_{\alpha-1}}{\partial x} + u\frac{\partial f_\alpha}{\partial x}\\ &\quad - \frac{\mathcal{T}^2}{2\rho}f_{\alpha-3}\frac{\partial \rho}{\partial x} - \frac{f_{\alpha-2}}{\rho}\frac{\partial q}{\partial x}\\ &\quad + \frac{1}{2\rho}(-2f_{\alpha-1} + \mathcal{T}f_{\alpha-3})\frac{\partial P}{\partial x}\\ &\quad = -V'(x)f_{\alpha-1}, \alpha = 0,\cdots,M\end{aligned} \tag{6}$$

Specifically,

$$f_0 = \rho, \quad f_1 = f_2 = 0, \quad P = \rho\mathcal{T}, \quad q = 3f_3. \tag{7}$$

As an example, the equations composing the regularized moment system corresponding to $M = 3$ is

$$\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial x} + \rho\frac{\partial u}{\partial x} = 0, \tag{8}$$

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$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+\frac{1}{\rho}\frac{\partial P}{\partial x}=-V'(x), \tag{9}$$

$$\frac{\partial P/2}{\partial t}+u\frac{\partial P/2}{\partial x}+\frac{3}{2}P\frac{\partial u}{\partial x}+3\frac{\partial f_3}{\partial x}=0, \tag{10}$$

$$\frac{\partial f_3}{\partial t}-\frac{P^2}{2\rho^2}\frac{\partial \rho}{\partial x}+\frac{P}{2\rho}\frac{\partial P}{\partial x}+u\frac{\partial f_3}{\partial x}=0. \tag{11}$$

The closure results for the collisionless BTE in a globally hyperbolic M-th order regularized moment system (6) can be organized into

$$\frac{\partial \boldsymbol{w}}{\partial t}+\mathbf{M}(\boldsymbol{w})\frac{\partial \boldsymbol{w}}{\partial x}=\mathbf{G}_f\boldsymbol{w}, \tag{12}$$

where $\boldsymbol{w}=(\rho,u,P/2,f_3,\cdots f_M)^T$ and $\mathbf{M}$, $\mathbf{G}$ corresponding to (8)-(11) are

$$\mathbf{M}=\begin{pmatrix} u & \rho & 0 & 0\\ 0 & u & \frac{2}{\rho} & 0\\ 0 & 3P & u & 3\\ -\frac{P^2}{2\rho^2} & 0 & \frac{P}{\rho} & u\end{pmatrix},$$

and

$$\mathbf{G}_f=\begin{pmatrix} 0 & 0 & 0 & 0\\ -\frac{V'(x)}{\rho} & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{pmatrix},$$

respectively. The characteristic velocities of (12) can be given exactly as $s_j=u+c_j\sqrt{\mathcal{T}},\quad j=1,2,\cdots,M+1$, where c_j is the j-th root of $H_{M+1}(x)$. In the moment framework, the scattering integral involving both the acoustical part and optical electron-phonon part are to be expressed into product of a scattering matrix $\mathbf{G}_{\text{scat}}$ and the expansion coefficient vector $\boldsymbol{F}=(f_0,f_1,\cdots,f_M)^T$, which lead to a moment system for the scattering by

$$\frac{\partial \boldsymbol{F}}{\partial t}=\mathbf{G}_{\text{scat}}\boldsymbol{F}. \tag{13}$$

$\mathbf{G}_{\text{scat}}=\mathbf{G}_{\text{ac}}+\mathbf{G}_{\text{op}}$, in which $\mathbf{G}_{\text{ac}}$ and $\mathbf{G}_{\text{op}}$ are the scattering matrices for the acoustic part and optical part respectively. Precisely, for the acoustic electron-phonon scattering

$$\mathbf{G}_{\text{ac}}(\alpha,\beta)=\begin{cases}\frac{\mathcal{T}^{\alpha/2}}{\alpha!}h_{\lfloor\frac{\alpha-1}{2}\rfloor,\lfloor\frac{\beta-1}{2}\rfloor} & \text{if } \alpha,\beta \text{ are odd,}\\ 0 & \text{else;}\end{cases}$$

where

$$h_{n,\beta}=\sum_{m=0}^{n}(-1)^{\beta+1}C_{2n+1,2m+1}2^{2\beta+m+\frac{7}{2}}\mathcal{T}^{-(\beta+1)}\pi^{-1}$$
$$\Gamma(m+1)\Gamma(\beta+\tfrac{3}{2})F(-\beta,m+1;\tfrac{3}{2};2), \tag{14}$$

where $F(\alpha,\beta;\gamma;z)$ is the Gauss hypergeometric function. For the optical electron-phonon scattering

$$\begin{aligned}&\mathbf{G}_{\text{op}}(2m,2\alpha)\\ &=\frac{\sqrt{\frac{8}{\pi}}\mathcal{T}^m}{(2m)!}\sum_{i=0}^{m}C_{2m,2i}\sum_{\beta=0}^{\alpha}\mathcal{T}^{-(\alpha+\beta+i+\frac{1}{2})}\\ &(2\hbar\omega_{op})^{i+\beta}C_{2\alpha,2\beta}(\exp(-\tfrac{\hbar\omega_{op}}{\mathcal{T}_L})I(2\beta,2i-1)\\ &-\exp(-\tfrac{\hbar\omega_{op}}{\mathcal{T}})I(0,2i+2\beta-1)\\ &+\exp(-\tfrac{\hbar\omega_{op}}{\mathcal{T}})I(2i,2\beta-1)\\ &-\exp(-\tfrac{\hbar\omega_{op}}{\mathcal{T}_L})I(2i+2\beta,-1)),\end{aligned} \tag{15}$$

and

$$\begin{aligned}&\mathbf{G}_{\text{op}}(2m+1,2\alpha+1)\\ &=-\frac{\sqrt{\frac{8}{\pi}}\mathcal{T}^{m+\frac{1}{2}}}{(2m+1)!}\sum_{i=0}^{m}C_{2m+1,2i+1}\sum_{\beta=0}^{\alpha}\mathcal{T}^{-(\alpha+\beta+i+2)}\\ &(2\hbar\omega_{op})^{i+\beta+1}C_{2\alpha+1,2\beta+1}(\exp(-\tfrac{\hbar\omega_{op}}{\mathcal{T}})I(0,2\beta+2i+1)\\ &+\exp(-\tfrac{\hbar\omega_{op}}{\mathcal{T}_L})I(2i+2\beta+2,-1)),\end{aligned} \tag{16}$$

where $\mathcal{T}_L$ is the lattice temperature and

$$\begin{aligned}I(m,n)&=\int_0^{+\infty}k^m\sqrt{k^2+1}^n\exp(-\frac{\hbar\omega_{op}}{\mathcal{T}}k^2)\,\mathrm{d}k\\ &=\frac{1}{2}\Gamma(\frac{m+1}{2})U(\frac{m+1}{2},\frac{m+n+3}{2},\frac{\hbar\omega_{op}}{\mathcal{T}}).\end{aligned} \tag{17}$$

As can be seen, all the elements of the scattering matrix $\mathbf{G}_{\text{scat}}$ are analytically expressed with the special functions, precisely, the Gamma function $\Gamma(x)$, the Gauss hypergeometric function $F(\alpha,\beta,\gamma;z)$ and the confluent hypergeometric function $U(a,b,z)$. Specifically, all of the elements of the first row of $\mathbf{G}_{\text{scat}}$ are zeros, which implies mass conservation is guaranteed during each collision. We have adopted the numerical method proposed in [5], [7] which is a unified numerical method for the moment system of arbitrary order. A time splitting method is used for the moment system derived from the BTE. The convection part is discretized by the finite volume method(FVM) with a HLL scheme for calculating the numerical flux, and the remaining scattering part is solved by the backward Euler scheme.

III. Results

Simulation of a 100-50-100(nm)'s n^+-n-n^+ SNW is carried out. The doping density of the Source/Drain region and the channel region are $5\times10^{17}\text{cm}^{-3}$ and $2\times10^{15}\text{cm}^{-3}$, respectively. The lattice temperature is fixed at 300K throughout the simulation process. A uniform mesh with a 0.5nm spacing is used in the x direction. Our simulations were performed for applied biases V_{bias} from 0V to 2.0V, but for the space saving, we only show I-V curves computed in the bias range $[0,1.0]$V. As is mentioned in [7], The numerical method designed for this globally hyperbolic moment method has the absolute predominance in CPU efficiency because the computation cost of this numerical method is only $\mathcal{O}(M/h)$, where h is the partition of the x-direction.

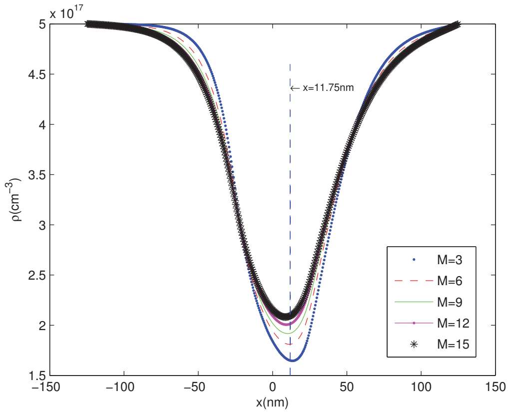

Fig. 1. The densities of the electron obtained at $M = 3, 6, 9, 12, 15$ respectively, where the cross points of the vertical dash line and the density curves are involved in the calculation of the relative errors.

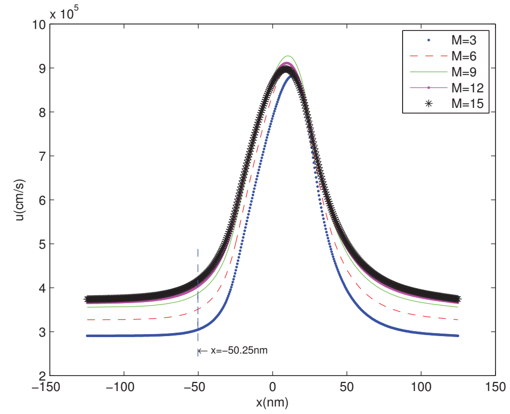

Fig. 2. the mean velocities of the electron obtained at $m = 3, 6, 9, 12, 15$ respectively, where the cross points of the vertical dash line and the mean velocity curves are involved in the calculation of the relative errors.

The convergence of all the macroscopic quantities with respect to the increase order of the moment system are plotted in Fig. 1, Fig. 2 and Fig. 3. The reference solutions for all the macroscopic quantities discussed in this paper are the numerical results calculated when $M = 15$. Apparently, with the increase of the number of the moments, the corresponding curves for all of the macroscopic quantities, densities, mean velocities and mean temperatures precisely, are getting close to the reference solutions.

The relative errors of all the macroscopic quantities at different observation points are plotted together in Fig: 4, in which $M \in [3, 10]$, $V_{bias} = 1.8$V. As expected, all of the macroscopic quantities considered in this paper are obviously convergent with the increase of the number of moments, and even present linear convergence rates.

As the most important characteristic curve of all semiconductor devices, I-V curves simulated when $M = 3$ and $M = 6$ are plotted in Fig. 5, and the significantly decrease in the current when increasing the bias shows the feasibility of our method. We show some curves of the mean velocity with

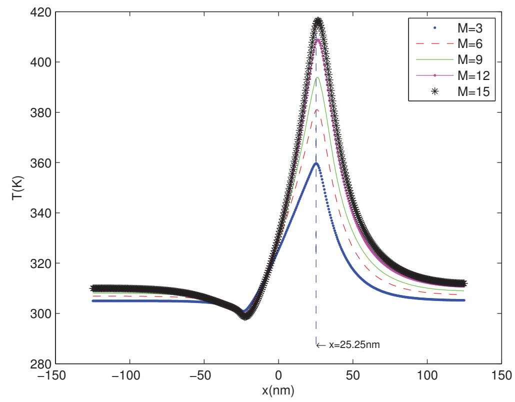

Fig. 3. The local temperatures of the electron obtained at $M = 3, 6, 9, 12, 15$ respectively, where the cross points of the vertical dash line and the local temperature curves are involved in the calculation of the relative errors.

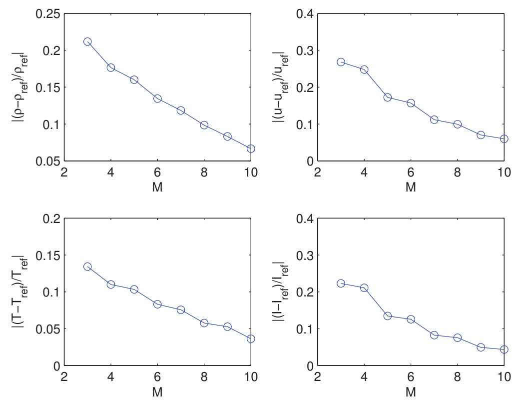

Fig. 4. The relative errors of electron's densities, mean velocities and local temperatures on the cross grids of the dash lines and the x-axis corresponding to Fig: 1, Fig: 2 and Fig: 3, respectively. The relative errors of average currents with respect to the moment order are plotted in the lower right subfig. The order set considered is $M \in [3, 10]$ and the reference is takes at $M = 15$. $V_{bias} = 1.8V$ is fixed throughout the whole calculation.

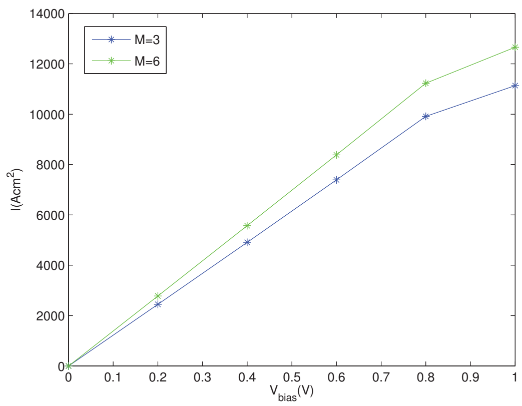

Fig. 5. I-V curves of $M = 3$ and $M = 6$ with the bias set is selected as $[0, 1.0]$V.

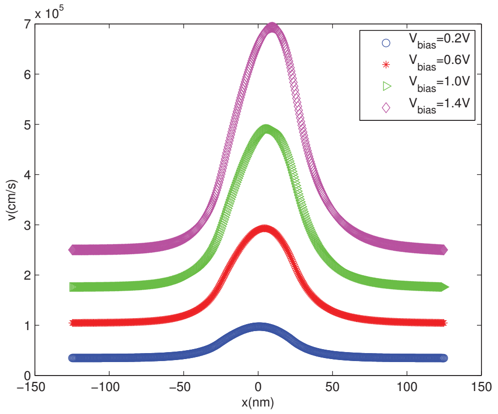

Fig. 6. The curves of mean velocities obtained when increasing biases applied with $M = 6$.

increasing biases in Fig. 6, in which M is fixed at 6. The mean velocity of electron obviously increases with the increase of the biases, which shows the rationality of our simulation.

IV. Conclusions

Globally hyperbolic moment systems of arbitrary order are systematically derived from the BTE including phonon-electron scattering. It is applied to simulate a 1-D SNW. Due to the globally hyperbolic regularization, the yielded moment system is well-posed. The convergence with respect to the order of the moment system is observed. Reasonable characteristics including I-V curves are obtained. The globally hyperbolic moment systems seem to be regarded as a series of high-order moment models as a good extension of the DD model.

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