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Stochastic Galerkin methods for the Boltzmann-Poisson system

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ABSTRACT

We study uncertainty quantification for a Boltzmann-Poisson system that models electron transport in semiconductors and the physical collision mechanisms over the charges, using the stochastic Galerkin method in order to handle the randomness associated with the problem. In this study we choose first as a source of uncertainty the phonon energy, taking it as a random variable, as its value influences the energy jump appearing in the collision integral for electron-phonon scattering. Then we choose the lattice temperature as a random variable, since it defines the value of the collision operator terms in the case of electron-phonon scattering by being a parameter of the phonon distribution. Finally, we present our numerical simulations for the latter case. We calculate then with our stochastic Discontinuous Galerkin methods the uncertainty in kinetic moments such as density, mean energy, current, etc. associated to a possible physical temperature variation (assumed to follow a uniform distribution) in the lattice environment, as this uncertainty in the temperature is propagated into the electron PDF. Our mathematical and computational results let us predict then in a real world problem setting the impact that possible variations in the lab conditions (such as temperature) or limitations in the mathematical model (such as assumption of a constant phonon energy) will have over the uncertainty in the behavior of electronic devices.

1. Introduction

1.1. The deterministic Boltzmann-Poisson system

Electronic transport in semiconductors is a problem that, although definitely quantum mechanical in nature, can be approximated up to a certain point by semiclassical models featuring quantum corrections. In the semiclassical modeling, even with deterministic laws of motion, the number of electric charge carriers $N \gg 1$ is of the order of the Avogadro number. The consequence is that a statistical model on the semiclassical scale is extremely adequate due to the large number of particles (i.e., the charge carriers, which are electrons in our problem), because it is virtually impossible to know exactly the initial conditions of positions and momentums for all the particles (on top of quantum considerations such as the Uncertainty Principle which indicate that knowing these initial conditions exactly is completely impossible). Therefore, uncertainty in the initial condition is naturally linked to the essence of the electron transport problem due to

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its many-carriers nature, even under a semiclassical approximation of this quantum problem, which consequently requires a statistical formulation, provided then by a particle density mechanics approach in terms of a probability density function in phase space. This probabilistic formulation is given precisely by the Boltzmann-Poisson (BP) semiclassical model for collisional electronic transport.

The Boltzmann-Poisson (BP) system for electron transport on a single conduction energy band has the form

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar}\nabla_{\vec{k}}\,\varepsilon(\vec{k}) \cdot \nabla_{\vec{x}} f - \frac{q}{\hbar}\vec{E}(\vec{x},t) \cdot \nabla_{\vec{k}} f = Q(f), \tag{1}$$

$$\nabla_{\vec{x}} \cdot (\epsilon\, \nabla_{\vec{x}} V) = q\left[\rho(\vec{x},t) - N(\vec{x})\right], \quad \vec{E} = -\nabla_{\vec{x}} V, \tag{2}$$

with the quantum mechanical electron group velocity $\frac{1}{\hbar}\nabla_{\vec{k}}\,\varepsilon(\vec{k})$, where $\varepsilon(\vec{k})$ is the conduction energy band structure function, $\epsilon = \epsilon(x)$ is the permittivity of the material, $N(x)$ is the doping density of positive charges assumed fixed in the material, $V = V(x,t)$ is the electric potential, and the electron density is $\rho(\vec{x},t) = \int_{\Omega_{\vec{k}}} f(\vec{x},\vec{k},t)\,d\vec{k}$. The collision integral operator $Q(f)$ describes the scattering over the electrons, where several mechanisms of quantum mechanical nature can be taken into account. In its full form, it enforces the Pauli Exclusion Principle by being given as

$$Q(f)(t,\vec{x},\vec{k}) = \int\limits_{\Omega_{\vec{k}'}} \left[S(\vec{k}' \to \vec{k}) f'(1-f) - S(\vec{k} \to \vec{k}') f (1-f')\right] d\vec{k}'. \tag{3}$$

The collision scattering term $S(\vec{k} \to \vec{k}'; \varepsilon(\vec{k}) \to \varepsilon(\vec{k}'))$ acts over f in our semiclassical model as a scattering matrix does in a quantum description over the wave function $\Psi(\vec{k})$ for a $\vec{k}$-state, i.e., representing the transition from a momentum $\vec{k}$ to another state $\vec{k}'$, satisfying momentum and energy conservation principles. There's then an analogy $\left\langle \Psi(\vec{k}) | S | \Psi(\vec{k}') \right\rangle \leftrightarrow \int_{\Omega_{\vec{k}'}} S(\vec{k}' \to \vec{k}) f'(1-f) d\vec{k}'$. It is important to mention that the specific form of $S(\vec{k} \to \vec{k}')$ can be derived from first-order time-dependent perturbation theory for the Schrödinger equation, by considering the perturbative Hamiltonian representing the scattering mechanisms under consideration. In the low density regime, however, we can relax the enforcing of the Pauli principle. In that case, the collisional integral operator can be approximated as being linear in f and therefore having the form

$$Q(f) = \int\limits_{\Omega_{\vec{k}}} \left[S(\vec{k}',\vec{k}) f(t,\vec{x},\vec{k}') - S(\vec{k},\vec{k}') f(t,\vec{x},\vec{k})\right] d\vec{k}', \tag{4}$$

where $S(\vec{k},\vec{k}') = S(\vec{k} \to \vec{k}')$ is the scattering kernel representing non-local interactions of electrons with a background density distribution. For example, in the case of silicon, the most important collision mechanisms are electron-phonon scatterings due to lattice vibrations of the crystal, which are modeled by acoustic (assumed elastic) and optical (non-elastic) non-polar modes, the latter with a single frequency ω_p (assumed constant), as in

$$\begin{aligned} S(\vec{k},\vec{k}') = {} & (n_q+1)\, K\, \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k}) + \hbar\omega_p) \\ & + n_q\, K\, \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k}) - \hbar\omega_p) + K_0\, \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k})), \end{aligned} \tag{5}$$

where K and K_0 are material constants for silicon. The symbol δ indicates the usual Dirac delta distribution, derived under the well-known Fermi's Golden Rule approximation in time-dependent perturbation theory [1]. The constant n_q is related to the phonon occupation factor

$$n_q(\hbar\omega_p) = \left[\exp\left(\frac{\hbar\omega_p}{K_B T_L}\right) - 1\right]^{-1}, \tag{6}$$

where K_B is the Boltzmann constant and $T_L = 300$ K is the lattice temperature.

1.2. Main uncertainties of the Boltzmann-Poisson model

We can summarize the main uncertainties of the Boltzmann-Poisson model for electron transport in semiconductors as follows.

1. The initial conditions for and the large number of particles of the system, leading to a probabilistic formulation of the problem in terms of $f(\vec{x},\vec{k},t)$.
2. Quantum mechanical features in the Boltzmann equation, particularly in the collision operator $Q(f)$, based on a probabilistic description of the electron as a wavefunction Ψ: $\left\langle \Psi_{\vec{k}} | S | \Psi_{\vec{k}'} \right\rangle \leftrightarrow \int_{\Omega_{\vec{k}'}} S(\vec{k}' \to \vec{k}) f'(1-f) d\vec{k}'$.

3. Uncertainty in the exact functional form of the energy band $\varepsilon(\vec{k})$. This function defines both the quantum terms of transport $\nabla_{\vec{k}}\varepsilon(\vec{k})$ and of electron-phonon scattering in silicon $\delta(\varepsilon(\vec{k}) - \varepsilon(\vec{k}') + l\hbar\omega_p)$, $l \in \{-1, 0, +1\}$, appearing in the Boltzmann equation.
4. The lattice temperature T may fluctuate, since it is related to the environmental temperature.
5. The phonon energy $\hbar\omega_p$ is often assumed to be constant, but it is known from experiments that this is not the case in general.
6. Parameters in the Poisson equation such as doping and permittivity may be uncertain. These are experimental parameters, and since they are given by measurements they are associated with measurement errors.
7. The boundary conditions that connect the domain to a stochastic environment. For example, reflection at physical boundaries might not be perfectly specular but rather have a diffusive component due to roughness in these boundaries.

In summary, uncertainty in the Boltzmann-Poisson system is crucial due to the practical impossibility to know precisely the initial condition of a classical system made of a number of particles of the order of the Avogadro number, which then uses the initial phase space density as an initial probability density function (in a probabilistic interpretation of this many particle problem), and also because strictly speaking the problem is of a quantum mechanical nature, where additionally, even the theoretical possibility of knowing precisely the initial condition of both position and momentum at the same time is prevented by Heisenberg's uncertainty principle.

1.3. The stochastic Boltzmann-Poisson system

Because of these reasons, we consider a stochastic Boltzmann-Poisson system of the form

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar}\nabla_{\vec{k}}\,\varepsilon(\vec{k},\vec{z})\cdot\nabla_{\vec{x}} f - \frac{q}{\hbar}\vec{E}(\vec{x},t,\vec{z})\cdot\nabla_{\vec{k}} f = Q(f)(t,\vec{x},\vec{k},\vec{z}), \tag{7}$$

$$\nabla_{\vec{x}}\cdot(\epsilon\,\nabla_{\vec{x}} V) = q\left[\rho(\vec{x},t) - N(\vec{x})\right], \quad \vec{E} = -\nabla_{\vec{x}} V, \tag{8}$$

with $f(t,\vec{x},\vec{k},\vec{z})$ being the probability density function now depending on an additional random parameter vector $\vec{z}$. The components of our random vector will be associated with the sources of uncertainty abovementioned, and they will be explicitly restated when we describe the stochastic Galerkin method for the Boltzmann-Poisson system.

1.4. Previous work on uncertainty quantification for Boltzmann models via stochastic Galerkin methods

We list below some references on the general UQ background and motivation relevant to our paper. We also make a brief presentation of existing results for UQ of Boltzmann kinetic models in particular, as well as work specifically related to Boltzmann-Poisson.

Regarding different UQ methodologies in general, we can think of Monte Carlo methods [2], stochastic collocation (SC) [3], general Polynomial Chaos - stochastic Galerkin (gPC-SG) [4], or Bayesian Estimation [5] with the cited references as some examples of sources for these different methods. An overview of several UQ approaches for hyperbolic and kinetic equations in particular can be found in [6], [7], [8], [9], [10], [11].

Regarding stochastic Galerkin (SG) methods specifically, in addition to its classical references, such as Wiener's polynomial chaos [12], Ghanem and Spanos [13], Xiu and Karniadakis [14], etc., SG for transport equations, and in particular for kinetic equations such as Boltzmann, has boomed relatively recently. It is a very active research area where both theoretical and computational results have been found in the last years. Some examples in the literature in this regard, related to transport and kinetic equations, can be found in [15], [16], [17], [18], [19], [20], [21], [22]. One of the first papers that considered the use of SG computations in the Boltzmann equation for gases was written by Hu and Jin [23]. Later on, SG was studied in the context of kinetic equations with random inputs, considering different models such as random linear and nonlinear Boltzmann equations, linear transport equations, and Vlasov-Poisson-Fokker-Planck equations. One of the studies on sG methods for the classical Boltzmann collision operator can be found in [22], where some results are presented as well on the consistency of a hybrid sG-based numerical method that preserves physical quantities. An overall view of the advances in the discipline for these equations can be found in the review paper [24], part as well of the review book [8].

More specifically, regarding SG methods for the semiconductor Boltzmann equation, one of the first works related to this topic was performed in [25]. They consider in their model a collision operator whose scattering kernel term is bounded above and below. Although uncertainties can possibly come from the collision operator, the electric potential, initial data, or boundary data, the collision operator in this previous study of the semiconductor Boltzmann equation did not consider the more physically realistic case of Dirac delta distributions obtained by Fermi's Golden Rule for energy transitions, as the scattering kernel was assumed to be bounded. Furthermore, a possible uncertainty in the electron velocity was not considered by making the assumption of a deterministic velocity given by the parabolic energy band model. Most importantly, the numerical study in this work considered a random relaxation Maxwellian collision kernel, which does not involve energy transitions in its scattering model, in addition to random initial data in the electron density, random boundary data, a random Debye length, and random doping parameters in the Poisson equation. Therefore, the randomness of the energy band in the transport and collision terms and the uncertainty related to a collision operator that uses Dirac delta distributions

due to Fermi's Golden Rule, as it is the case for electron-phonon scattering, remain as crucial topics yet to be studied for the understanding of uncertainty quantification in collisional electron transport in semiconductors via stochastic methods. Some other relevant works related to SG methods for the Boltzmann-Poisson system in semiconductors are, for example, [18], [26]. However, similar assumptions in the bounding above and below of the collision kernel (and sometimes its derivatives too) are made in these works. Then, the problem of studying a collision kernel involving the Dirac delta remains as an interesting problem to be examined. Our methodology will then be to study variables related to the electron-phonon collision operator as random in the SG method for the Boltzmann-Poisson model of electrons in semiconductors. We first choose as one of those variables the lattice temperature, as it is involved in the phonon distribution as a parameter. The dimensional cost is minimal as the temperature is a scalar.

We describe the structure of the rest of this paper as follows. In Section 2 we discuss how the SG method handles the uncertainties arising in the Boltzmann-Poisson system. Then we consider uncertainty quantification by SG first for the phonon energy being a random variable and then the lattice temperature being a random variable too. Section 3 describes the numerics of the deterministic Boltzmann-Poisson system solved by discontinuous-Galerkin (DG) methods. Then Section 4 covers in more detail the stochastic discontinuous Galerkin (SDG) method for the Boltzmann-Poisson system for the case of a random lattice temperature. In Section 5, the conclusions are drawn.

2. Stochastic Galerkin method for the Boltzmann-Poisson system

2.1. Description of uncertainties

The SG method handles the uncertainties in the Boltzmann-Poisson system by introducing random variables z_i, $i \in \{1, \ldots, 7\}$, associated with the uncertainties as indicated below.

1. Regarding initial conditions and the large number of particles, the probabilistic formulation $f(\vec{x}, \vec{k}, t, z_1)$ with random initial conditions $f(\vec{x}, \vec{k}, 0, z_1)$ is used.
2. Regarding quantum phenomena in the collision operator $Q(f)$, the probabilistic nature of the electron wavefunction Ψ is mimicked (relaxing Pauli principle) by $\langle \Psi_{\vec{k}'} | S | \Psi_{\vec{k}} \rangle \leftrightarrow \int_{\Omega_{\vec{k}}} S(\vec{k} \to \vec{k}', z_2) f(\vec{x}, \vec{k}, t, z_2) d\vec{k}'$.
3. The uncertainty in the energy band structure is described as $\varepsilon(\vec{k}, z_3)$. This function defines both quantum terms of electron velocity $\nabla_{\vec{k}} \varepsilon(\vec{k}, z_3)/\hbar$ and of electron-phonon scattering in silicon $\delta(\varepsilon(\vec{k}, z_3) - \varepsilon(\vec{k}', z_3) + l(\hbar\omega_p + z_4))$, $l \in \{-1, 0, +1\}$.
4. The lattice temperature is written as $T + z_4$ as it may change due to fluctuations in the environment, but it is assumed to be constant in the model.
5. The phonon energy $\hbar\omega_p + z_5$ is approximated as constant in the model, but experiments show that it is nonconstant in general.
6. In the Poisson equation, the doping concentration is written as $N_D + z_6$ and the permittivity as $\epsilon + z_6$.
7. The boundary conditions are described as $f_B(\vec{x}, \vec{k}, t, z_7)|_{\partial\Omega}$, etc.

2.2. Stochastic Galerkin method for the Boltzmann-Poisson system with the phonon energy as a random variable

In this section, we assume that the only uncertainty stems from the phonon energy model. Randomness in the phonon energy is physically relevant because it is known to be strictly speaking non-constant, and it is also a good starting point as a scalar random variable. Therefore, we replace $\hbar\omega_p$ in the deterministic equation by $\hbar\omega_p + z$. Then the phonon occupation as a function of the energy becomes

$$n_q(\hbar\omega_p, z) = \left[\exp\left(\frac{\hbar\omega_p + z}{K_B T_L} \right) - 1 \right]^{-1}. \tag{9}$$

This introduces randomness in the collision operator as well, leading to

$$\begin{aligned} S(\vec{k}, \vec{k}', z) = &\left[n_q(\hbar\omega_p, z) + 1 \right] K \, \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k}) + \hbar\omega_p + z) \\ + K_0 \, \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k})) + &n_q(\hbar\omega_p, z) \, K \, \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k}) - \hbar\omega_p - z). \end{aligned}$$

We consider two cases. First we devise a stochastic Galerkin algorithm using a distributional-derivative approximation with respect to the random variable. Then we consider the fully general case of the random variable in the collision operator without any distributional-derivative approximation in the random space. The algorithms are described in detail in the following.

2.2.1. Random phonon energy using a distributional derivative approximation

We consider the approximation of the phase space density (with $\vec{p} = \hbar\vec{k}$ being the crystal momentum) by a general truncation of order K,

$$f(t,\vec{x},\vec{p},z) \approx f_K(t,\vec{x},\vec{p},z) = \sum_{k=1}^{K} \alpha_k(t,\vec{x},\vec{p})\Psi_k(z) = \alpha(t,\vec{x},\vec{p})\cdot\Psi(z), \tag{10}$$

$$\alpha(t,\vec{x},\vec{p}) = (\alpha_1,\cdots,\alpha_n), \quad \Psi(z) = (\Psi_1,\cdots,\Psi_n), \tag{11}$$

where $\{\Psi_k(z)\}_{k=1}^{\infty}$ is defined as the basis orthonormal with respect to the distribution of uncertainty $\pi(z)$ for the random variable z. That is, we have that

$$\delta_{km} = \int_{\Omega_z} \Psi_k(z)\Psi_m(z)\pi(z)dz. \tag{12}$$

We note that Ψ_k depends on only one z_i, $i = 1, ..., 7$, only if the uncertainties are independent.
For the case $n := 1$, $P := 1$, $K := \dim(\mathcal{P}_P^n) := 2$, and then

$$f(t,\vec{x},\vec{p},z) \approx \sum_{k=1}^{2} \alpha_k(t,\vec{x},\vec{p})\Psi_k(z) = \alpha(t,\vec{x},\vec{p})\cdot\Psi(z) = (\alpha_1,\alpha_2)\cdot(\Psi_1,\Psi_2), \tag{13}$$

then the Boltzmann equation reads

$$\partial_t\alpha + \vec{v}\cdot\nabla_{\vec{x}}\alpha + F\cdot\nabla_{\vec{p}}\alpha = Q(\alpha), \tag{14}$$

$$Q(\alpha) = \int_{\Omega_{\vec{p}}} B(\vec{p},\vec{p}')[M(\vec{p})\alpha(\vec{p}') - M(\vec{p}')\alpha(\vec{p})]d\vec{p}', \tag{15}$$

$$B_{ij}(\vec{p},\vec{p}') = \int_{I_z} \sigma(\vec{p},\vec{p}',z)\Psi_i(z)\Psi_j(z)\pi(z)dz \tag{16}$$

$$= \sigma_0(\vec{p},\vec{p}')\delta_{ij} + \int_{I_z} \partial_z\sigma(\vec{p},\vec{p}',z)|_{z=0} z\Psi_i(z)\Psi_j(z)\pi(z)dz, \tag{17}$$

$$\sigma(\vec{p},\vec{p}',z) = \sigma_0(\vec{p},\vec{p}') + \tilde{\sigma}_1(\vec{p},\vec{p}')z = \sigma|_{z=0} + \partial_z\sigma(\vec{p},\vec{p}',z)|_{z=0}z. \tag{18}$$

The collision scattering cross section is then written as

$$\sigma(\vec{p},\vec{p}',z) = \sigma_0(\vec{p},\vec{p}') + \tilde{\sigma}_1(\vec{p},\vec{p}')z, \tag{19}$$

which we have assumed is the main source of uncertainties in the studied problem, therefore the partial dependence of $\sigma(\vec{p},\vec{p}',z)$ on the random variable z, and where we also have

$$\sigma_0 = M^{-1}[K_0\delta(\varepsilon-\varepsilon') + (e^{\hbar\omega_p}-1)^{-1}K(e^{\hbar\omega_p}\delta(\varepsilon-\varepsilon'+\hbar\omega_p) + \delta(\varepsilon-\varepsilon'-\hbar\omega_p))]. \tag{20}$$

Here $\tilde{\sigma}_1(\vec{p},\vec{p}') = \partial_z\sigma(\vec{p},\vec{p}',z)|_{z=0}$ is a distributional derivative with respect to z, and we find

$$\tilde{\sigma}_1(\vec{p},\vec{p}') = M^{-1}K\partial_z\Big\{[1+(e^{\hbar\omega_p+z}-1)^{-1}]\delta(\varepsilon-\varepsilon'+\hbar\omega_p+z) + (e^{\hbar\omega_p+z}-1)^{-1}\delta(\varepsilon-\varepsilon'-\hbar\omega_p-z)\Big\}|_{z=0}.$$

Using $\delta'[\phi] = -\delta[\phi']$ and phonon distribution properties, we have

$$\tilde{\sigma}_1(\vec{p},\vec{p}') = M^{-1}K\Big\{[1+(e^{\hbar\omega_p}-1)^{-1}]\partial_z|_0\delta(\varepsilon-\varepsilon'+\hbar\omega_p+z) + (e^{\hbar\omega_p}-1)^{-1}\partial_z|_0\delta(\varepsilon-\varepsilon'-\hbar\omega_p-z) - \frac{e^{\hbar\omega_p}}{(e^{\hbar\omega_p}-1)^2}[\delta(\varepsilon-\varepsilon'+\hbar\omega_p)+\delta(\varepsilon-\varepsilon'-\hbar\omega_p)]\Big\}$$

and

$$B_{ij}(\vec{p},\vec{p}') = \sigma_0(\vec{p},\vec{p}')\delta_{ij} + M^{-1}K\int_{I_z} dz\Psi_i(z)\Psi_j(z)\pi(z)z\cdot \cdot\Big\{[1+(e^{\hbar\omega_p}-1)^{-1}]\partial_z|_0\delta(\varepsilon-\varepsilon'+\hbar\omega_p+z)$$

$$
\begin{aligned}
&+ (e^{\hbar\omega_p} - 1)^{-1}\partial_z|_0\delta(\varepsilon - \varepsilon' - \hbar\omega_p - z) \\
&- \frac{e^{\hbar\omega_p}}{(e^{\hbar\omega_p} - 1)^2}[\delta(\varepsilon - \varepsilon' + \hbar\omega_p) + \delta(\varepsilon - \varepsilon' - \hbar\omega_p)]\Big\} \\
&= \sigma_0(\vec{p}, \vec{p'})\delta_{ij} - M^{-1}K \cdot \\
&\cdot\Big\{[1 + (e^{\hbar\omega_p} - 1)^{-1}]\partial_z[\Psi_i(z)\Psi_j(z)\pi(z)z]\chi|_{z=-(\varepsilon-\varepsilon'+\hbar\omega_p)} \\
&+ (e^{\hbar\omega_p} - 1)^{-1}\partial_z[\Psi_i(z)\Psi_j(z)\pi(z)z]\chi|_{z=+(\varepsilon-\varepsilon'-\hbar\omega_p)} \\
&+ \frac{e^{\hbar\omega_p}\int_{I_z} dz\Psi_i(z)\Psi_j(z)\pi(z)z}{(e^{\hbar\omega_p} - 1)^2}\sum_{\pm}\delta(\varepsilon - \varepsilon' \pm \hbar\omega_p)\Big\}.
\end{aligned}
$$

We explain some concrete examples of distributions of the random variable for this problem in Appendix A.

2.2.2. Random phonon energy without a distributional derivative approximation in the random space

Next, we consider again a random phonon energy, but now use the collision scattering term without approximation by distributional derivatives in the random space. For a general truncation, we recall from 2.2.1 that we would have

$$f(t, \vec{x}, \vec{p}, z) \approx f_K(t, \vec{x}, \vec{p}, z) = \sum_{k=1}^{K}\alpha_k(t, \vec{x}, \vec{p})\Psi_k(z) = \alpha(t, \vec{x}, \vec{p}) \cdot \Psi(z), \tag{21}$$

$$\alpha(t, \vec{x}, \vec{p}) = (\alpha_1, \cdots, \alpha_n), \quad \Psi(z) = (\Psi_1, \cdots, \Psi_n). \tag{22}$$

We consider again the case $n := 1$, $P := 1$, $K := \dim(\mathcal{P}_P^n) := 2$, and approximate the density again as

$$f(t, \vec{x}, \vec{p}, z) \approx \sum_{k=1}^{2}\alpha_k(t, \vec{x}, \vec{p})\Psi_k(z) = \alpha(t, \vec{x}, \vec{p}) \cdot \Psi(z) = (\alpha_1, \alpha_2) \cdot (\Psi_1, \Psi_2). \tag{23}$$

Then the Boltzmann equation reads

$$\partial_t\alpha + v \cdot \nabla_{\vec{x}}\alpha + F \cdot \nabla_{\vec{p}}\alpha = Q(\alpha), \tag{24}$$

$$Q(\alpha) = \int_{\Omega_p} B(\vec{p}, \vec{p'})[M(\vec{p})\alpha(\vec{p'}) - M(\vec{p'})\alpha(\vec{p})]d\vec{p'}, \tag{25}$$

$$B_{ij}(\vec{p}, \vec{p'}) = \int_{I_z} \sigma(\vec{p}, \vec{p'}, z)\Psi_i(z)\Psi_j(z)\pi(z)dz, \tag{26}$$

$$\sigma(\vec{p}, \vec{p'}, z) = \frac{K_0\delta(\varepsilon - \varepsilon') + K\frac{e^{\beta(\hbar\omega_p+z)}\delta(\varepsilon-\varepsilon'+\hbar\omega_p+z)+\delta(\varepsilon-\varepsilon'-\hbar\omega_p-z)}{e^{\beta(\hbar\omega_p+z)}-1}}{M(\vec{p})} \tag{27}$$

with $\beta = (K_B T_L)^{-1}$. We then have

$$B_{ij}(\vec{p}, \vec{p'}) = \frac{K_0\delta(\varepsilon - \varepsilon')\delta_{ij} + K\int_{I_z} dz\Psi_i(z)\Psi_j(z)\pi(z)\left\{\frac{e^{\beta(\hbar\omega_p+z)}\delta(\varepsilon-\varepsilon'+\hbar\omega_p+z)+\delta(\varepsilon-\varepsilon'-\hbar\omega_p-z)}{e^{\beta(\hbar\omega_p+z)}-1}\right\}}{M(\vec{p})}.$$

Therefore, we find

$$B_{ij}(\vec{p}, \vec{p'}) = \frac{K_0\delta(\varepsilon - \varepsilon')\delta_{ij} + K\left(\frac{\chi(z)\Psi_i(z)\Psi_j(z)\pi(z)e^{\beta(\hbar\omega_p+z)}}{e^{\beta(\hbar\omega_p+z)}-1}\Big|_{z=\varepsilon'-\varepsilon-\hbar\omega_p} + \frac{\chi(z)\Psi_i(z)\Psi_j(z)\pi(z)}{e^{\beta(\hbar\omega_p+z)}-1}\Big|_{z=\varepsilon-\varepsilon'-\hbar\omega_p}\right)}{M(\vec{p})}$$

with $\chi(z)$ being the characteristic function. Furthermore, we have

$$
\begin{aligned}
B = {} & M^{-1}(\vec{p})K_0\delta(\varepsilon - \varepsilon')I \\
& + \frac{\frac{K\chi(z)\pi(z)}{1-e^{-\beta(\hbar\omega p+z)}}\begin{pmatrix}\Psi_1^2(z) & \Psi_1\Psi_2\\ \Psi_1\Psi_2 & \Psi_2^2(z)\end{pmatrix}\Big|_{\varepsilon'-\varepsilon-\hbar\omega_p} + \frac{K\chi(z)\pi(z)}{e^{\beta(\hbar\omega p+z)}-1}\begin{pmatrix}\Psi_1^2(z) & \Psi_1\Psi_2\\ \Psi_1\Psi_2 & \Psi_2^2(z)\end{pmatrix}\Big|_{\varepsilon-\varepsilon'-\hbar\omega_p}}{M(\vec{p})}.
\end{aligned}
$$

We write the specifics of this problem for the particular case of a uniform distribution for the random variable in Appendix A as well.

2.3. Stochastic Galerkin method for the Boltzmann-Poisson system with the lattice temperature as a random variable

In this example, we assume that the only uncertainty in our problem stems from the lattice temperature. Randomness in the lattice temperature is motivated by physical reasons, as the temperature in the material or in its environment often fluctuates. The random variable is scalar, and randomness is introduced in the collisions, but now outside the argument of the Dirac delta distributions associated with Fermi's Golden Rule.

Therefore, the term $K_B T_L$ in the deterministic equation is replaced by $K_B T_L + z^*$, or equivalently, the term $\beta := (K_B T_L)^{-1}$ in the deterministic equation is replaced by $\beta + z$. This introduces randomness in the phonon occupation as a function the energy, yielding

$$n_q(\hbar\omega_p, z) = \left[\exp\left(\frac{\hbar\omega_p}{K_B T_L + z^*}\right) - 1\right]^{-1} = \left[e^{(\beta+z)\hbar\omega_p} - 1\right]^{-1}. \tag{28}$$

Additionally, randomness in the collision operator model is introduced as well. We have

$$\begin{aligned} S(\vec{k}, \vec{k}', z) &= \left[n_q(\hbar\omega_p, z) + 1\right] K\, \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k}) + \hbar\omega_p) \\ &+ K_0\, \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k})) + n_q(\hbar\omega_p, z)\, K\, \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k}) - \hbar\omega_p). \end{aligned}$$

Noticing that the randomness is just in the coefficients related to the phonon density and not inside the arguments of the delta distributions, we equivalently have

$$\begin{aligned} S(\vec{k}, \vec{k}', z) &= K\, \frac{e^{(\beta+z)\hbar\omega_p}}{e^{(\beta+z)\hbar\omega_p} - 1}\, \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k}) + \hbar\omega_p) \\ &+ K_0\, \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k})) + K\, \frac{1}{e^{(\beta+z)\hbar\omega_p} - 1}\, \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k}) - \hbar\omega_p). \end{aligned}$$

In particular, we consider the random temperature $T_L + z$, set $n := 1$, $P := 1$, $K := \dim(\mathcal{P}_P^n) = 2$, and approximate the density as

$$f(t, \vec{x}, \vec{p}, z) \approx \sum_{k=1}^{2} \alpha_k(t, \vec{x}, \vec{p})\Psi_k(z) = \alpha(t, \vec{x}, \vec{p}) \cdot \Psi(z) = (\alpha_1, \alpha_2) \cdot (\Psi_1, \Psi_2). \tag{29}$$

This yields the Boltzmann equation

$$\partial_t \alpha + v \cdot \nabla_{\vec{x}} \alpha + F \cdot \nabla_{\vec{p}} \alpha = Q(\alpha), \tag{30}$$

$$Q(\alpha) = \int_{\Omega_p} B(\vec{p}, \vec{p}')[M(\vec{p})\alpha(\vec{p}') - M(\vec{p}')\alpha(\vec{p})]d\vec{p}', \tag{31}$$

$$B_{ij}(\vec{p}, \vec{p}') = \int_{I_z} \sigma(\vec{p}, \vec{p}', z)\Psi_i(z)\Psi_j(z)\pi(z)dz \tag{32}$$

with the scattering cross section

$$\sigma(\vec{p}, \vec{p}', z) = \frac{1}{M(\vec{p})}\left(K_0\delta(\varepsilon - \varepsilon') + K\frac{e^{(\beta+z)\hbar\omega_p}\delta(\varepsilon - \varepsilon' + \hbar\omega_p) + \delta(\varepsilon - \varepsilon' - \hbar\omega_p)}{e^{(\beta+z)\hbar\omega_p} - 1}\right). \tag{33}$$

Substituting σ into B_{ij} yields

$$\begin{aligned} B_{ij}(\vec{p}, \vec{p}') &= \int_{I_z} dz\Psi_i(z)\Psi_j(z)\pi(z)\frac{K_0\delta(\varepsilon - \varepsilon') + K\frac{e^{(\beta+z)\hbar\omega_p}\delta(\varepsilon-\varepsilon'+\hbar\omega_p)+\delta(\varepsilon-\varepsilon'-\hbar\omega_p)}{e^{(\beta+z)\hbar\omega_p}-1}}{M(\vec{p})} \\ &= M^{-1}(\vec{p})K_0\delta(\varepsilon - \varepsilon')\delta_{ij} + \int_{I_z} dz\Psi_i(z)\Psi_j(z)\pi(z)\frac{K\frac{e^{(\beta+z)\hbar\omega_p}\delta(\varepsilon-\varepsilon'+\hbar\omega_p)+\delta(\varepsilon-\varepsilon'-\hbar\omega_p)}{e^{(\beta+z)\hbar\omega_p}-1}}{M(\vec{p})}. \end{aligned}$$

This expression simplifies to

$$B_{ij}(\vec{p}, \vec{p}') = \frac{K_0\delta(\varepsilon - \varepsilon')\delta_{ij} + K\left(\delta(\varepsilon - \varepsilon' + \hbar\omega_p)\int_{I_z}\frac{dz\Psi_i\Psi_j\pi}{1-e^{-(\beta+z)\hbar\omega_p}} + \delta(\varepsilon - \varepsilon' - \hbar\omega_p)\int_{I_z}\frac{dz\Psi_i\Psi_j\pi}{e^{(\beta+z)\hbar\omega_p}-1}\right)}{M(\vec{p})}$$

and

$$B_{ij}(\vec{p},\vec{p'}) = M(\vec{p})^{-1}\left[K_0\delta(\varepsilon-\varepsilon')\delta_{ij} + K\left(\delta(\varepsilon-\varepsilon'+\hbar\omega_p)C_{ij}^{+} + \delta(\varepsilon-\varepsilon'-\hbar\omega_p)C_{ij}^{-}\right)\right]$$

with the coefficients

$$C_{ij}^{-} = \int_{I_z} dz\Psi_i(z)\Psi_j(z)\pi(z)\frac{1}{e^{(\beta+z)\hbar\omega_p}-1} = \int_{I_z} dz\Psi_i(z)\Psi_j(z)\pi(z)\,n_q(\hbar\omega_p,\beta+z),$$

$$C_{ij}^{+} = \int_{I_z} dz\Psi_i(z)\Psi_j(z)\pi(z)\left(1+\frac{1}{e^{(\beta+z)\hbar\omega_p}-1}\right) = \int_{I_z} dz\Psi_i\Psi_j\pi\left(n_q+1\right) = \delta_{ij} + C_{ij}^{-}.$$

Therefore the scattering operator becomes

$$\begin{aligned} Q(\alpha) &= \int_{\Omega_{\vec{p}}}\left(K_0\delta(\varepsilon-\varepsilon')I_d + K\sum_{\pm}\delta(\varepsilon-\varepsilon'\pm\hbar\omega_p)C^{\pm}\right)M(\vec{p})^{-1}\left[M(\vec{p})\alpha(\vec{p'}) - M(\vec{p'})\alpha(\vec{p})\right]d\vec{p'} \\ &= \int_{\Omega_{\vec{p}}}\left(\sum_{l=-1}^{1}K_l\delta(\varepsilon-\varepsilon'+l\hbar\omega_p)C^{l}\right)M(\vec{p})^{-1}\left[M(\vec{p})\alpha(\vec{p'}) - M(\vec{p'})\alpha(\vec{p})\right]d\vec{p'} \end{aligned}$$

with $K_{-1} = K = K_{+1}$ and $C_{ij}^{0} = \delta_{ij}$ being the identity matrix.

It is important to note that a Gaussian distribution is not appropriate in this example, as there would arise a singularity in the integrals when the temperature (in energy units) becomes zero. We hence assume a uniform distribution $\pi(z) = N/2\beta$ for $z\in[-\beta/N,\beta/N]$ with $N>1$, or equivalently $\pi(w)=1/2$ by the scaling $w = Nz/\beta$ for $w\in[-1,1]$, with the associated Legendre polynomials $\Psi_1 = 1$ and $\Psi_2(w) = w$. This means that $f\approx\alpha_1 + w\alpha_2$. Therefore we find

$$C^{-} = \int_{-\beta/N}^{\beta/N}\frac{dz\,N/2\beta}{e^{(\beta+z)\hbar\omega_p}-1}\begin{pmatrix}1 & Nz/\beta\\ Nz/\beta & (Nz/\beta)^2\end{pmatrix} = \frac{1}{2}\int_{-1}^{1}\frac{\begin{pmatrix}1 & w\\ w & w^2\end{pmatrix}dw}{e^{\beta\hbar\omega_p(1+w/N)}-1}.$$

The analytic values of these integrals are

$$\begin{aligned} \int\frac{dx}{\exp(A+Bx)-1} &= \frac{\log(1-e^{A+Bx})}{B} - x + ct,\\ \int\frac{xdx}{\exp(A+Bx)-1} &= \frac{\mathrm{Li}_2(e^{A+Bx})}{B^2} + \frac{x\log(1-e^{A+Bx})}{B} - \frac{x^2}{2} + ct,\\ \int\frac{x^2dx}{\exp(A+Bx)-1} &= \frac{-2\mathrm{Li}_3(e^{A+Bx})}{B^3} + \frac{2x\mathrm{Li}_2(e^{A+Bx})}{B^2} + \frac{x^2\log(1-e^{A+Bx})}{B} - \frac{x^3}{3} + ct \end{aligned}$$

with $A = \beta\hbar\omega_p$, $B = \beta\hbar\omega_p/N$, and $\mathrm{Li}_n(x)$ being the polylogarithm functions. Furthermore, we can evaluate these formulas to obtain C^{-} explicitly in the form

$$C^{-} = \frac{1}{2}\begin{pmatrix}\frac{\log(1-e^{A+Bx})}{B} - x\Big|_{-1}^{1} & \frac{\mathrm{Li}_2(e^{A+Bx})}{B^2} + \frac{x\log(1-e^{A+Bx})}{B}\Big|_{-1}^{1}\\ \frac{\mathrm{Li}_2(e^{A+Bx})}{B^2} + \frac{x\log(1-e^{A+Bx})}{B}\Big|_{-1}^{1} & \frac{-2\mathrm{Li}_3(e^{A+Bx})}{B^3} + \frac{2x\mathrm{Li}_2(e^{A+Bx})}{B^2} + \frac{x^2\log(1-e^{A+Bx})}{B} - \frac{x^3}{3}\Big|_{-1}^{1}\end{pmatrix},$$

where we can omit the term $-\frac{x^2}{2}$ in the off-diagonal elements, since it will vanish when evaluating at ±1.

To determine concrete numbers for numerical simulations and for the evaluation of the C^{-} matrix, we recall that the Planck constant divided by 2π is equal to $\hbar = h/2\pi = 1.0546\times10^{-34}$ J·s and that the Boltzmann constant is equal to $K_B = 1.3805\times10^{-23}$ J/K. The mean lattice temperature is assumed to be $T_L := 300$ K $= 26.85\,^{\circ}$C. Therefore, we have that $K_BT_L = 4.1415\times10^{-21}$ J $= 0.025\,849$ eV, since 1 eV $= 1.602\,18\times10^{-19}$ J. Hence $\beta = (K_BT_L)^{-1} = 2.414\,584\,1\times10^{20}$ J^{-1}.

Moreover, the variation in the environment temperature might be of $\pm10\,^{\circ}$C, resulting in a lattice temperature between $16.85\,^{\circ}$C $= 290$ K and $36.85\,^{\circ}$C $= 310$ K. In that case $K_BT_L\in[4.003\,45, 4.279\,55]\times10^{-21}$ J, $\beta+z\in[2.336\,694\,3, 2.497\,845\,6]\times10^{20}$ J^{-1}, and $z\in[-0.077\,889\,8, 0.083\,261\,5]\times10^{20}$ J^{-1}. Thus $z\in I_z$, which is $I_z\approx[-0.080\,575\,65, 0.080\,575\,65]\times10^{20}$ J^{-1}, and therefore $\beta/N = 0.080\,575\,65\times10^{20}$ J^{-1} implies $N = \frac{2.414\,584\,1\times10^{20}\ \mathrm{J}^{-1}}{0.080\,575\,65\times10^{20}\ \mathrm{J}^{-1}} = 29.966\,672\,313\,5$. After rounding to $N := 30$, we have $z\in[-\beta/N,\beta/N]$ with $\beta/N = 0.080\,486\,136\,66\times10^{20}$ J^{-1}. Finally, since the phonon energy is $\hbar\omega_p = 0.063$ eV $= 1.009\,373\,4\times10^{-20}$ J, we obtain the values of the adimensional numbers $\beta\hbar\omega_p = 2.437\,216\,962\,6 = A$ and $\beta\hbar\omega_p/N = 0.081\,240\,565\,42 = B$.

Hence we find the matrices

$$C^- = \frac{1}{2}\begin{pmatrix} 0.191\,825 & -0.005\,690\,12 \\ -0.005\,690\,12 & 0.064\,015\,1 \end{pmatrix} = \begin{pmatrix} 0.095\,912\,5 & -0.002\,845\,06 \\ -0.002\,845\,06 & 0.032\,007\,55 \end{pmatrix},$$
$$C^+ = \begin{pmatrix} 1.095\,912\,5 & -0.002\,845\,06 \\ -0.002\,845\,06 & 1.032\,007\,55 \end{pmatrix},$$

since $C^+_{ij} = C^-_{ij} + \delta_{ij}$. With these matrices, the scattering operator becomes

$$Q(\alpha) = \int_{\Omega_{\vec{p}}} \left(K_0 \delta(\varepsilon - \varepsilon') I_d + K \sum_{\pm} \delta(\varepsilon - \varepsilon' \pm \hbar\omega_p) C^{\pm} \right) \frac{M\alpha' - M'\alpha}{M} d\vec{p}', \tag{34}$$

which we can write in the form

$$Q(\alpha) = \int_{\Omega_{\vec{p}}} \left(K_0 \delta(\varepsilon - \varepsilon') + K \sum_{\pm} \delta(\varepsilon - \varepsilon' \pm \hbar\omega_p) \left[n_q + (1 \pm 1)/2 \right] \right) I_d \frac{M\alpha' - M'\alpha}{M} d\vec{p}'$$
$$+ \int_{\Omega_{\vec{p}}} K \left[\sum_{\pm} \delta(\varepsilon - \varepsilon' \pm \hbar\omega_p) \right] \left(C^- - n_q I_d \right) \frac{M\alpha' - M'\alpha}{M} d\vec{p}',$$

since $C^+ = C^- + I_d$ and hence $C^- - n_q I_d = C^+ - (n_q + 1) I_d$.

Therefore the term in the first row is the collision operator, as originally written in the deterministic case, acting on each separate band (by means of the identity matrix) without any recombination, whereas the second term represents the recombination and diagonal terms related to the uncertainty in the temperature associated solely with inelastic integrals. Given the value of the constant $n_q = \left[e^{\beta\hbar\omega_p} - 1 \right]^{-1} = 0.095\,774\,842\,71$, we find

$$C^- - n_q I_d = \begin{pmatrix} 0.000\,137\,657\,29 & -0.002\,845\,06 \\ -0.002\,845\,06 & -0.063\,767\,292\,71 \end{pmatrix} = C^+ - (n_q + 1) I_d.$$

3. Stochastic Galerkin method for the Boltzmann-Poisson system using deterministic discontinuous Galerkin solvers

The numerics of deterministic solvers for the Boltzmann-Poisson system that use the discontinuous Galerkin (DG) algorithm have been studied in [27], [28] for a single PDF (one band) without randomness. We will use the deterministic DG method for two bands (representing the α vector of coefficients) to solve the stochastic Galerkin system, which contains a different kind of matrix integral collisional operator.

3.1. Discontinuous Galerkin: the Boltzmann equation in $\vec{k}$-spherical coordinates

We perform a spherical transformation of the momentum coordinate $\vec{k}$ taking the location of a (local) minimum of the conduction energy band as the origin. This transformation is useful (in the absence of Umklapp effects), because in low energy limits (i.e., for small potential bias) the conduction band energy scales as the square of the momentum norm, and hence the radial coordinate is an energy variable. We then have

$$\vec{k} = \frac{\sqrt{2m^* K_B T_L}}{\hbar} \sqrt{r} \left(\mu, \sqrt{1-\mu^2}\cos\varphi, \sqrt{1-\mu^2}\sin\varphi \right),$$
$$r \geq 0, \qquad \mu \in [-1, 1], \qquad \varphi \in [-\pi, \pi],$$

where r is a normalized square of the momentum wavevector norm, $\mu = \cos(\theta)$ is the cosine of the polar angle θ, and φ is the azimuthal angle in the spherical coordinate $\vec{k}$-transformation. The variable r is proportional to the energy for small biases in the parabolic band approximation, assuming the same effective mass in all three Cartesian momentum directions. Due to this momentum coordinate transformation, we have to weight the PDF coefficients by the Jacobian of the $\vec{k}$-transformation, specifically for the computation of moment integrals over the $\vec{k}$-space. We then obtain a transformed PDF in the phase space $(\vec{x}, r, \mu, \varphi)$ given by

$$\Phi(t, \vec{x}, r, \mu, \varphi) = \frac{\sqrt{r}}{2} \alpha(t, \vec{x}, \vec{k}(r, \mu, \varphi)).$$

We also obtain a transformed Boltzmann equation in divergence form for our new PDF Φ in the $(x, y, z; r, \mu, \varphi)$ space, which reads

$$\frac{\partial \Phi}{\partial t} + \frac{\partial}{\partial x}(a_1\,\Phi) + \frac{\partial}{\partial y}(a_2\,\Phi) + \frac{\partial}{\partial z}(a_3\,\Phi) + \frac{\partial}{\partial r}(a_4\,\Phi) + \frac{\partial}{\partial \mu}(a_5\,\Phi) + \frac{\partial}{\partial \varphi}(a_6\,\Phi) = C(\Phi),$$

where the transport coefficients are, for $(a_1, a_2, a_3) \propto \nabla_{\vec{k}}\varepsilon(\vec{k})$, proportional to the $\vec{k}$-gradient in transformed coordinates, and the rest are given by

$$a_4 = -2\,c_E\,\sqrt{r}\,\hat{e}_r \cdot \underline{\mathrm{E}} = -2\,c_E\,\sqrt{r}\left(\mu, \sqrt{1-\mu^2}\cos\varphi, \sqrt{1-\mu^2}\sin\varphi\right)\cdot \underline{\mathrm{E}}, \tag{35}$$

$$a_5 = -c_E\frac{\sqrt{1-\mu^2}}{\sqrt{r}}\,\hat{e}_\mu \cdot \underline{\mathrm{E}} = -c_E\frac{\sqrt{1-\mu^2}}{\sqrt{r}}\left(\sqrt{1-\mu^2}, -\mu\cos\varphi, -\mu\sin\varphi\right)\cdot \underline{\mathrm{E}},$$

$$a_6 = -c_E\,\frac{1}{\sqrt{r}\sqrt{1-\mu^2}}\,\hat{e}_\varphi \cdot \underline{\mathrm{E}} = -c_E\,\frac{1}{\sqrt{r}\sqrt{1-\mu^2}}\,(0, -\sin\varphi, \cos\varphi)\cdot \underline{\mathrm{E}}. \tag{36}$$

Regarding the transformed linear collision operator, we write $\vec{x} = (x, y, z)$ and $\mathbf{r} = (r, \mu, \varphi)$, and obtain

$$C(\Phi)(t, \vec{x}, \mathbf{r}) = \frac{\sqrt{r}}{2}\int_\Omega \mathcal{S}(\mathbf{r}', \mathbf{r})\;\Phi(t, \vec{x}, \mathbf{r}')\,d\mathbf{r}' - \Phi(t, \vec{x}, \mathbf{r})\int_\Omega \mathcal{S}(\mathbf{r}, \mathbf{r}')\,\frac{\sqrt{r'}}{2}\,d\mathbf{r}',$$

showing the importance of the transformed PDF Φ. Here $\mathcal{S}(\mathbf{r}', \mathbf{r})$ represents the scattering for the two-band system, as presented in subsections 2.2 and 2.3.

We use the dimensionless Poisson equation

$$\nabla_{\vec{x}} \cdot (\epsilon_r \nabla_{\vec{x}} \Psi) = c_p\left[\rho(t, \vec{x}) - \mathcal{N}_D(\vec{x})\right], \tag{37}$$

where

$$\mathcal{N}_D(\vec{x}) = \left(\frac{\sqrt{2\,m^* K_B T_L}}{\hbar}\right)^{-3} N_D(\vec{x}), \tag{38}$$

and the electron density, as we only need it for the electric field, is approximated by the numerical value given by the first PDF coefficient,

$$\rho(t, \vec{x}) \approx \int_{\Omega_{\vec{k}}} f_1(t, \vec{x}, \vec{p}')d\vec{p}' = \Psi_1(z)\int_{\Omega_{\vec{k}}} \alpha_1(t, \vec{x}, \vec{p}')d\vec{p}' = 1 \cdot \int_\Omega \Phi_1(t, \vec{x}, \mathbf{r}')\,d\mathbf{r}', \tag{39}$$

which represents the mean of the density, as in

$$\rho(t, \vec{x}) = \frac{\int_{\Omega_z} \rho(t, \vec{x}, z)dz}{\int_{\Omega_z} dz} = \frac{\int_{\Omega_z}\int_{\Omega_{\vec{p}}} f(t, \vec{x}, \vec{p}, z)d\vec{p}dz}{\int_{\Omega_z} dz}.$$

The discontinuous Galerkin method for the Boltzmann-Poisson system represents a dynamic extension of the Gummel iteration map. Starting with an initial condition Φ_h and given boundary conditions, the DG algorithm advances from t^n to t^{n+1} in these steps:

Step 1 Compute the charge density ρ.
Step 2 Use ρ to solve the Poisson equation (either by an integral form in 1D or by the LDG method in 2D or 3D) for the potential and electric field, and compute the transport coefficients a_i, $1 \le i \le 6$.
Step 3 Solve the transport part of the Boltzmann equation by DG, then use the method of lines for Φ_h (ODE system).
Step 4 Evolve the ODE system by proper time stepping from t^n to t^{n+1} (if partial time steps are necessary, as in a Runge-Kutta method, repeat steps 1 to 3 as needed).

We use a rectangular Cartesian grid in the transformed phase space. It has the form

$$\Omega_{ijkmn} = \left[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}\right] \times \left[y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}}\right] \times \left[r_{k-\frac{1}{2}}, r_{k+\frac{1}{2}}\right] \times \left[\mu_{m-\frac{1}{2}}, \mu_{m+\frac{1}{2}}\right] \times \left[\varphi_{n-\frac{1}{2}}, \varphi_{n+\frac{1}{2}}\right]$$

with $1 \le i \le N_x$, $1 \le k \le N_r$, $1 \le m \le N_\mu$, and $x_{i\pm\frac{1}{2}} = x_i \pm \Delta x_i/2$, $r_{k\pm\frac{1}{2}} = r_k \pm \Delta r_k/2$, $\mu_{m\pm\frac{1}{2}} = \mu_m \pm \Delta\mu_m/2$.

The test functions $\psi(x, y, r, \mu, \varphi) \in V_h$ belong to the set of piecewise linear polynomials

$$V_h := V_h^l := \left\{v : v|\Omega_{ijkmn} \in P(\Omega^l_{ijkmn})\right\},$$

where the $P(\Omega^l_{ijkmn})$ are the polynomials of degree $l \leq 1$ on Ω_{ijkmn}.

Inside the cell $\mathring{\Omega}_I$, $I = (i, j, k, m, n)$, we approximate the weighted PDF by a linear polynomial in V_h componentwise,

$$\Phi_h = (\Phi_{1,h}, \Phi_{2,h}) = (\Phi_{q,h}), \quad q = 1, 2, \tag{40}$$
$$\Phi_{q,h} = T^q_I(t) + X^q_I(t)\,\frac{(x - x_i)}{\Delta x_i/2} + Y^q_I(t)\,\frac{(y - y_j)}{\Delta y_j/2} + R^q_I(t)\,\frac{(r - r_k)}{\Delta r_k/2} + M^q_I(t)\,\frac{(\mu - \mu_m)}{\Delta \mu_m/2} + P^q_I(t)\,\frac{(\varphi - \varphi_n)}{\Delta \varphi_n/2}.$$

In summary, the discontinuous Galerkin formulation for the vector Boltzmann equation is to find $\Phi_{q,h}$ in the piecewise polynomial space V_h, $q = 1, 2$, such that the equation

$$\begin{aligned}
&\int_K \frac{\partial \Phi_{q,h}}{\partial t} v_h d\Omega - \int_K \frac{\partial v_h}{\partial x}\left(a_1\,\Phi_{q,h}\right) d\Omega - \int_K \frac{\partial v_h}{\partial y}\left(a_2\,\Phi_{q,h}\right) d\Omega - \int_K \frac{\partial v_h}{\partial z}\left(a_3\,\Phi_{q,h}\right) v_h d\Omega \\
&- \int_K \frac{\partial v_h}{\partial r}\left(a_4\,\Phi_{q,h}\right) d\Omega - \int_K \frac{\partial v_h}{\partial \mu}\left(a_5\,\Phi_{q,h}\right) d\Omega - \int_K \frac{\partial v_h}{\partial \varphi}\left(a_6\,\Phi_{q,h}\right) d\Omega \\
&+ F^+_x - F^-_x + F^+_y - F^-_y + F^+_z - F^-_z + F^+_r - F^-_r + F^+_\mu - F^-_\mu + F^+_\varphi - F^-_\varphi = \int_K [C(\Phi_h)]_q v_h d\Omega,
\end{aligned}$$

where the $F^\pm$ represent the boundary integrals, holds for any test function $v_h \in V_h$ and for each element $K = \Omega_{ijkmn}$. In the equation above, $\int_K [C(\Phi_h)]_q d\Omega$ refers to the q-th row of the collision term in our multi-band Boltzmann system of equations.

4. SDG-BP: stochastic discontinuous Galerkin method for the Boltzmann-Poisson system

4.1. The symmetric case: one-dimensional in x, two-dimensional in $\vec{k}(r, \mu)$

We consider a 1D n^+–n–n^+ silicon diode, rendering the problem one-dimensional in position space. The length of the diode is $L = 1$ µm, and the length of the n-channel in the middle is 400 nm. The doping concentration is $n^+ = 5 \cdot 10^{23}/\mathrm{m}^3 = 5 \cdot 10^{17}/\mathrm{cm}^3$ and $n = 2 \cdot 10^{21}/\mathrm{m}^3 = 2 \cdot 10^{15}/\mathrm{cm}^3$.

We consider the case with k-space azimuthal symmetry on $\varphi \in [0, 2\pi] \to \vec{k} = \vec{k}(r, \mu)$. Therefore, by the symmetry assumptions, it is only necessary to consider the radial and polar coordinates of the momentum.

The computational domain is taken as $x \in [0, 1]$, $r \in [0, r_{\max}]$, and $\mu \in [-1, 1]$. The constant $r_{\max}$ is the cut-off such that $\Phi(t, x, r, \mu) \approx 0$ for $r \geq r_{\max}$ in the numerical experiments. For example, $r_{\max} \approx 36$ for $V_{\text{bias}} = 0.5$ V in a 400 nm channel.

The initial condition is $(\Phi_0, \Phi_1)(0, x, r, \mu) = (CN_D(x)e^{-\varepsilon(r)}\sqrt{r}/2, 0)$ with a constant C such that $\rho(0, x) - N_D(x) = 0$ at the initial time $t = 0$.

The boundary conditions are the following.

- In the x-space, the charge concentration is neutral at the source and drain endpoints $0 = x_{1/2}$ and $x_{N_x+1/2} = 1$. This charge neutrality condition is imposed by $\Phi(0, \vec{k}, t) = N_D(x)\frac{\Phi(x_1, \vec{k}, t)}{\rho(x_1, \vec{k}, t)}$ and $\Phi(1, \vec{k}, t) = N_D(x)\frac{\Phi(x_{N_x}, \vec{k}, t)}{\rho(x_{N_x}, \vec{k}, t)}$.
- The applied potential (bias) is $V(0, \vec{k}, t) = 0$ and $V(1, \vec{k}, t) = V_0$.
- In the (r, μ)-space, a cut-off boundary is used such that Φ vanishes at $r = r_{\max}$.
- At the "point" boundaries, no boundary conditions are needed and transport equals zero analytically. Hence, at the origin $r = 0$, $a_4 = 0$ holds, and likewise at the poles $\mu = \pm 1$, $a_5 = 0$ holds. Therefore the boundary integrals are analytically equal to zero at $r = 0$ and $\mu = \pm 1$.

Regarding time evolution, an RK2 Method was used in our simulations.

4.2. Numerical results

We present the numerical results for the coefficients of the truncated PDF with a random variable. We first do so for the benchmark case of no recombination DG-BP: $-\log \alpha_0(x, r, \mu)$ (and $\alpha_1(x, r, \mu) = 0$ plotted directly) are shown for a 1 µm diode, 0.5 V bias, and $t_0 = 10.0$ ps. In this deterministic case, the reason why there is no recombination lies in the vanishing of the first coefficient $\alpha_1 = 0$ related to random effects (Fig. 2), and the zeroth coefficient α_0 contains all the information of the PDF (Fig. 1).

We then consider the PDF coefficients from the simulations of the SDG-BP system with the recombination terms $-\log \alpha_0(x, r, \mu, t)$ in Fig. 3 and $-\log \alpha_1(x, r, \mu, t)$ in Fig. 4 for a 1 µm diode, 0.5 V bias, and $t_0 = 10.0$ ps as well. The variations in α_1 are located in similar regions of the phase space, while for α_0 they seem finer and more pronounced. (See also Figs. 5, 6.)

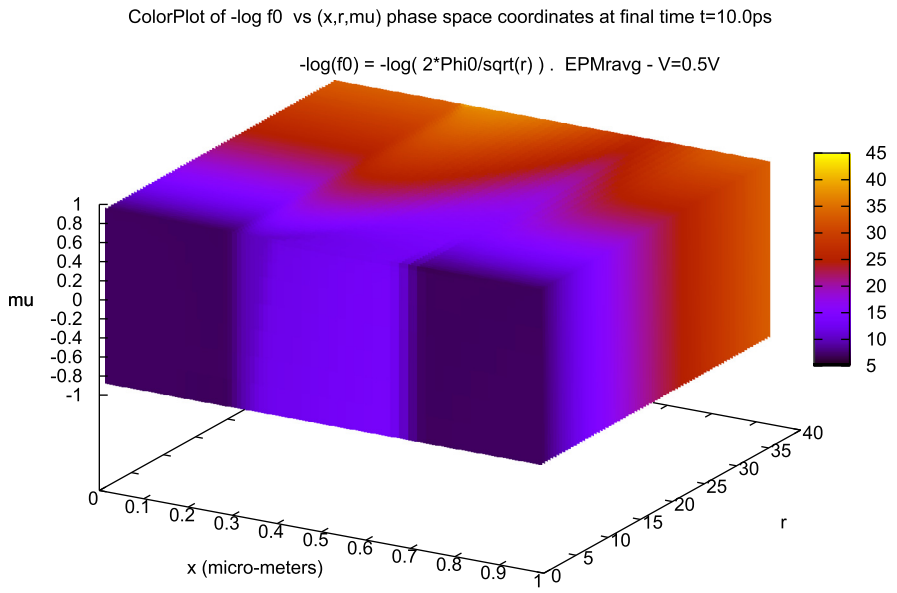

Fig. 1. $-\log\alpha_0(x,r,\mu)$ for a 1 μm diode, 0.5 V bias, and $t_0 = 10.0$ ps. (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

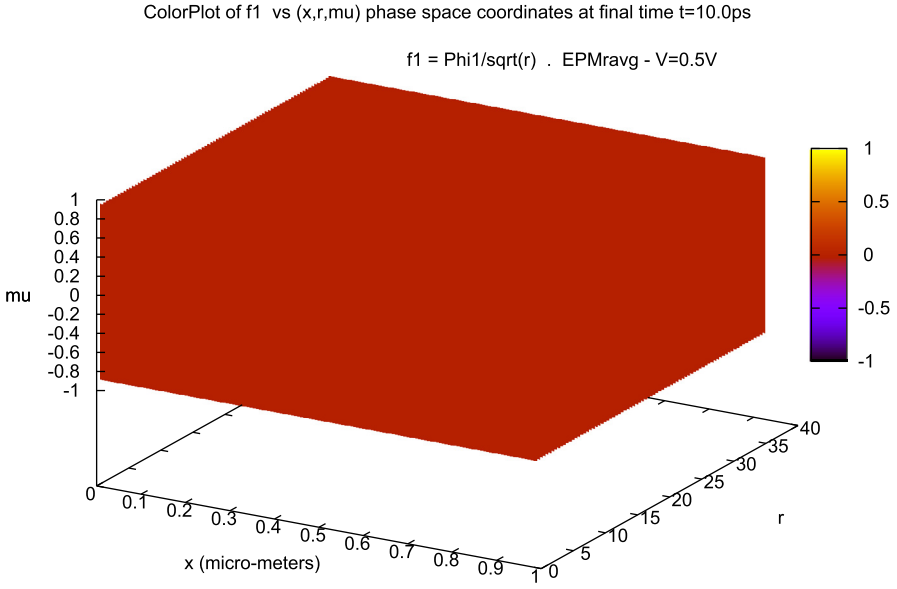

Fig. 2. Coefficient $\alpha_1(x,r,\mu) = 0$ for a 1 μm diode, 0.5 V bias, and $t_0 = 10.0$ ps.

We also compare SDG-BP with recombination terms against SDG-BP with no recombination case by calculating the moments with Φ_0 for both. The difference is observed mainly in the prediction of the momentum (current) two orders of magnitude below the mean value of the current (Fig. 11), indicating the finer resolution of the momentum by use of the stochastic Galerkin method. We also plot the expectation, variance, and standard deviation of our probability density function in the SDG-BP method, given as $\mathrm{E}[f] = \alpha_1$, $\mathrm{Var}[f] = \sum_{k=2}^{2} \alpha_k^2 = \alpha_2^2$, and $\mathrm{S}[f] = \sqrt{\sum_{k=2}^{2} \alpha_k^2} = |\alpha_2|$, respectively. (See Figs. 7–14.)

4.2.1. Study of convergence in the random space

We proceed to present our results of a numerical investigation performed in order to study the convergence in the random space of our stochastic Discontinuous Galerkin scheme.

Due to the lack of a known analytical solution to our time-dependent problem, we proceed to compare our solution with a reference solution obtained by means of a high-order (HO) stochastic collocation (SC) method [2,3,25]. This stochastic

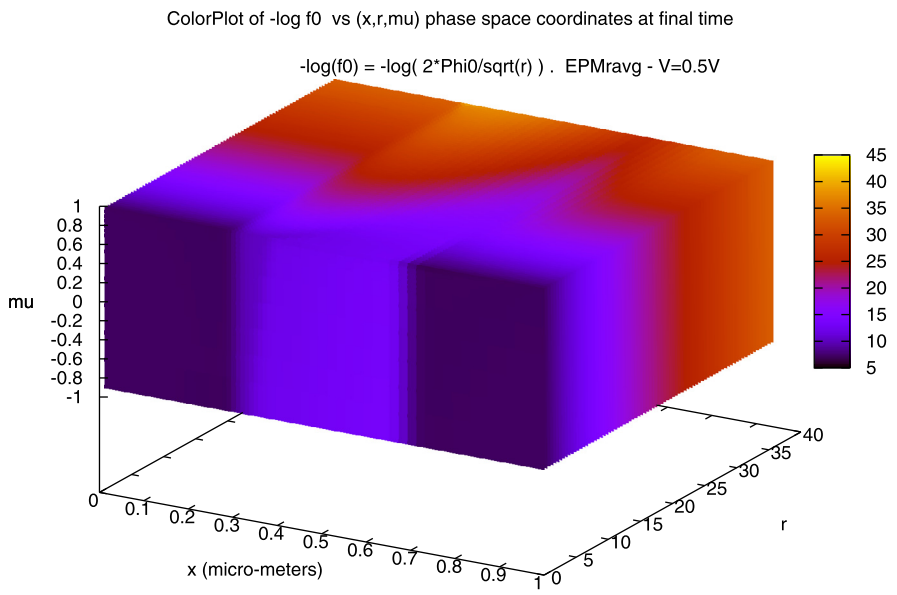

Fig. 3. $-\log\alpha_0(x, r, \mu)$ for a 1 μm diode, 0.5 V bias, and $t_0 = 10.0$ ps.

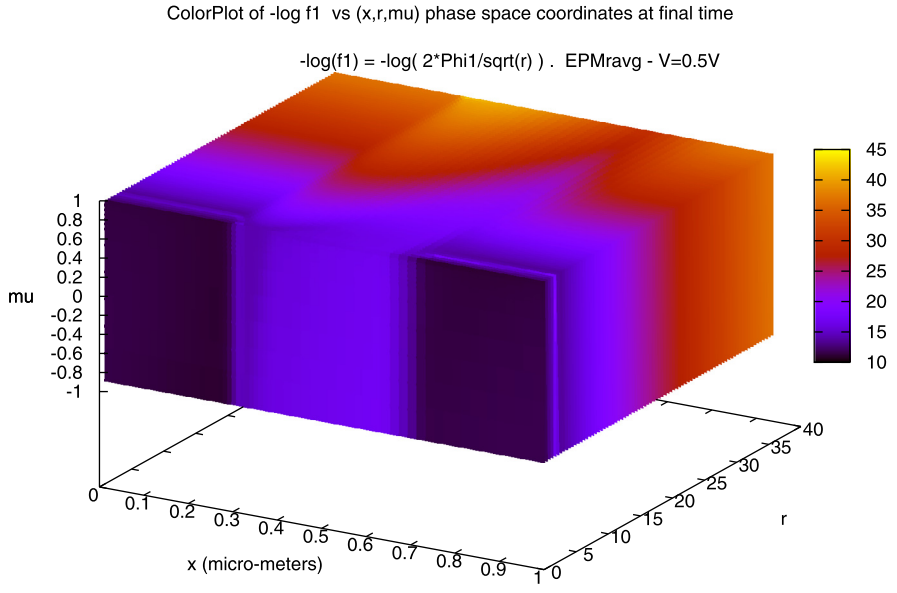

Fig. 4. $-\log\alpha_1(x, r, \mu)$ for a 1 μm diode, 0.5 V bias, and $t_0 = 10.0$ ps.

solution is obtained by averaging the results of 16 different deterministic simulations, each one corresponding to a different quadrature point for the study of randomness in the temperature. We take a uniform distribution around the mean value for the temperature, namely

$$T(z) = 300 + 10z, \quad z \in [-1, 1], \tag{41}$$

where the temperature units are Kelvins, to give the variation of ± 10 Kelvins around the mean value. In summary, the stochastic collocation takes N_z samples (in our case $N_z = 16$), each one corresponding to a different collocation node $z^{(j)}, 1 \leq j \leq N_z$, with $z^{(j)} \in [-1, 1] = I_z$. For each value $z^{(j)}$ of our samples, corresponding to a fixed value of a collocation node, we run a simulation of the deterministic Boltzmann-Poisson original problem. Once we have the different solutions $f(\vec{x}, \vec{k}, t, z^{(j)})$, we will interpolate to construct a stochastic approximation to the solution, namely

$$f(\vec{x}, \vec{k}, t, z) = \sum_{j=1}^{N_z} f(\vec{x}, \vec{k}, t, z^{(j)}) l_j(z), \tag{42}$$

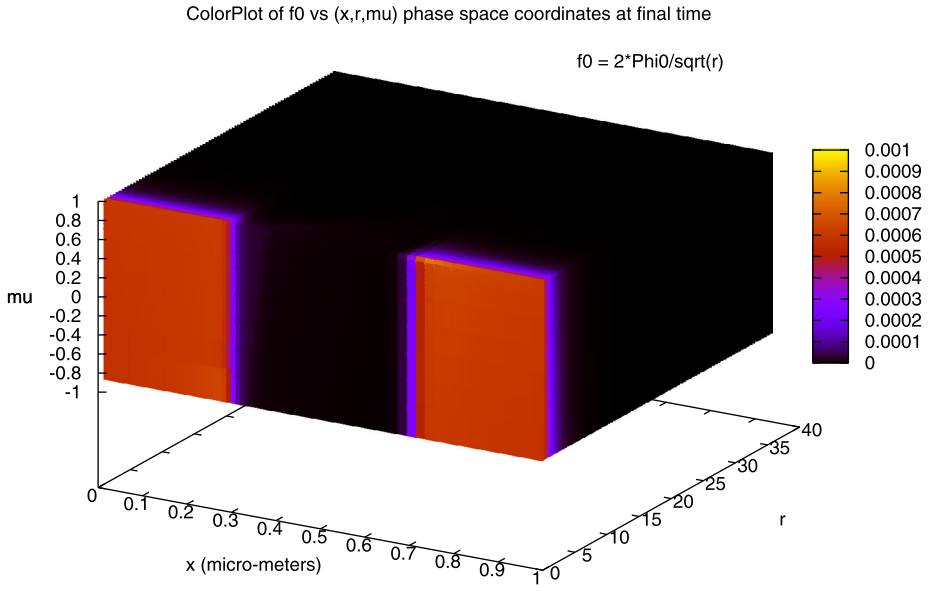

Fig. 5. Coefficient $\alpha_0(x, r, \mu)$ for a 1 µm diode, 0.5 V bias, and $t_0 = 10.0$ ps.

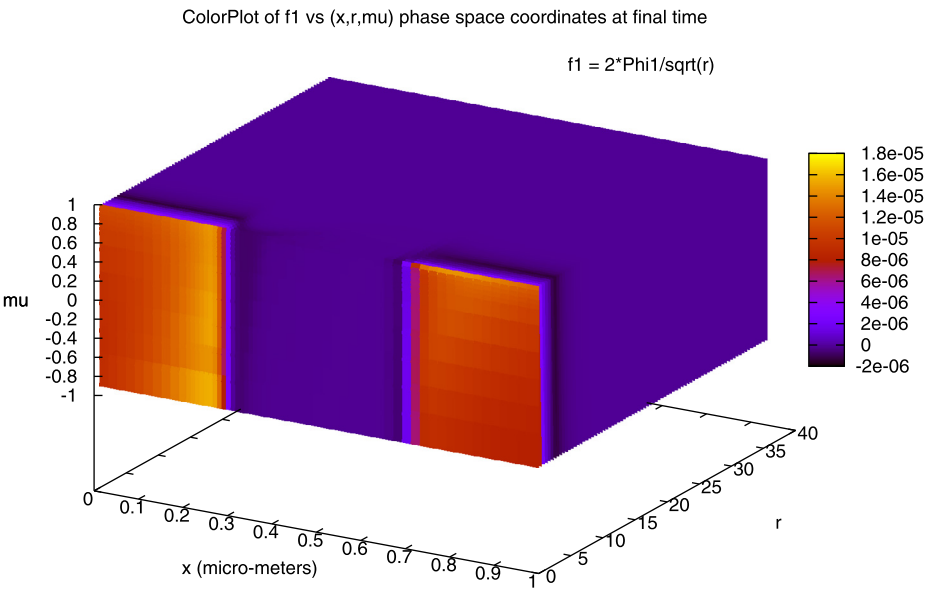

Fig. 6. Coefficient $\alpha_1(x, r, \mu)$ for a 1 µm diode, 0.5 V bias, and $t_0 = 10.0$ ps.

with $\{l_j(z)\}_{j=1}^{N_z}$ a truncated basis of functions corresponding to the probability distribution of choice for the problem. In our case, since a uniform distribution was chosen, a Lagrange interpolant having as nodes the zeros of the respective Legendre polynomials of degree N_z (since a gPC basis of Legendre polynomials corresponds to a uniform distribution) was used as basis in the interpolation process. More information about stochastic collocation can be found in [2,3].

We compare then our high-order stochastic collocation (HO-SC) solution obtained by means of 16 quadrature points with our stochastic Galerkin (sG) solution. In particular, we will compare the mean and standard deviation (the solution statistics) for a macroscopic physical quantity such as the density. We present in Figs. 15 and 16 the plots of the mean and standard deviation, respectively, for the density of both the sG solution and the HO-SC average solution (obtained by quadrature of 16 points) at different times in our evolution problem. Notice there's a difference of at least two orders of magnitude between the maximum values of the mean density in Fig. 15 and the density standard deviation in Fig. 16.

The mean density matches between the sG and HO-SC solutions over time, staying relatively constant over the evolution of the problem. The density standard deviation only changes slightly for the HO-SC solution during the time evolution, having two peaks localized close to the junction points $x = 0.3$, 0.7 microns, but for the sG solution, although it has peak

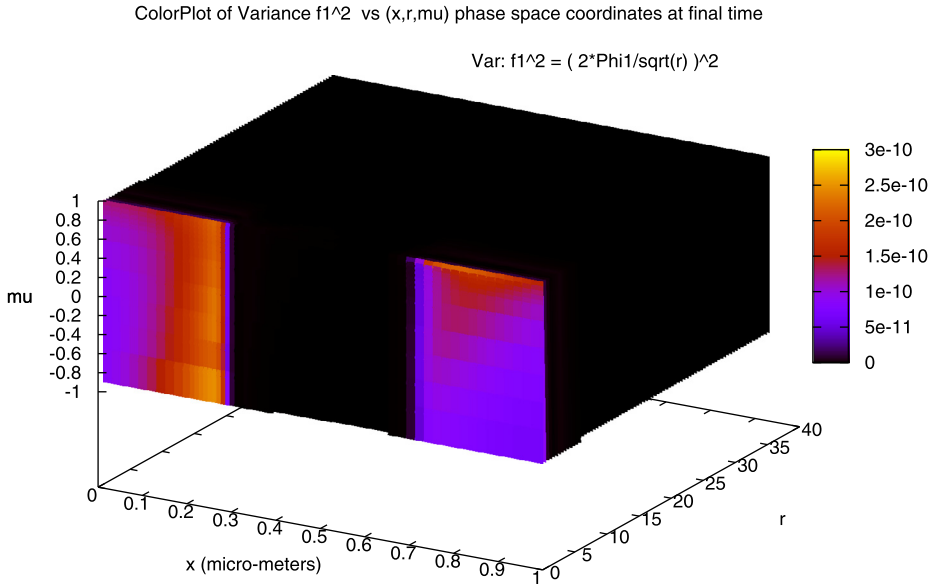

Fig. 7. Variance $\mathrm{Var}[f] = \alpha_2^2$.

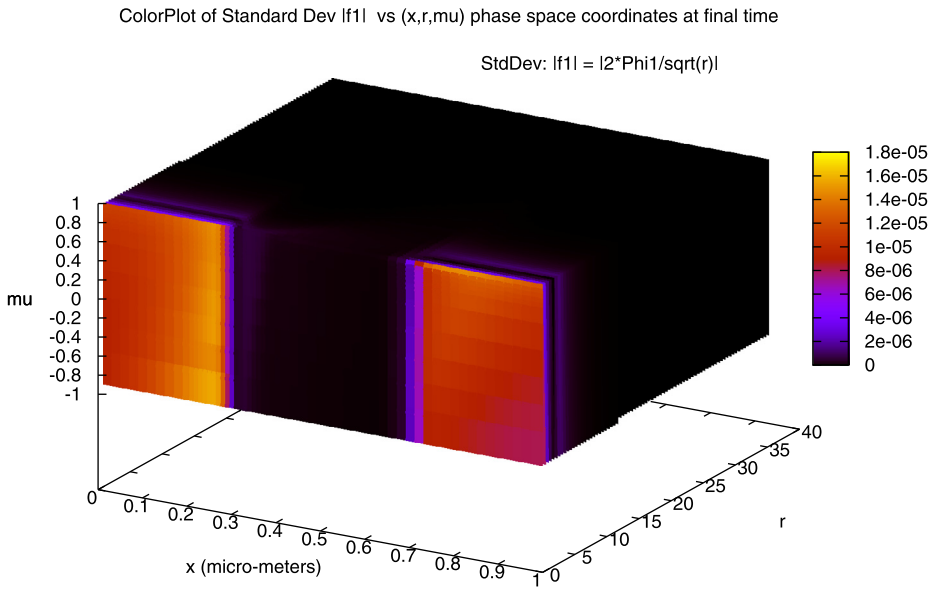

Fig. 8. Standard deviation $\mathrm{S}[f] = |\alpha_2|$.

heights close to the HO-SC ones at the time of $t = 1.25$ ps (with a greater width though), its peaks and their width grow with time, eventually having a nonzero standard deviation at the boundary points corresponding to $x = 0,\ 1$ microns.

We attribute the difference in the predictions for the standard deviation of the density to the truncation of the sG solution to only two bands. An increase in the number of elements of the sG basis could increase the closeness in the random space of the sG solution to the HO-SC reference solution, but coming at the cost of greater computational time for the solution of a system of more than two bands.

We proceed to present a complementary study of convergence with respect to the random variable z. We use again as a reference solution one obtained via a High-Order Stochastic Collocation approach with $N_{\max} = 16 = 2^4$ sample points, as in [25], in the absence of analytic solutions for our problem. We computed the L_2-errors for the density mean & standard deviation and for the transformed PDF $\Phi = \frac{\sqrt{r}}{2} f$ versus the reference solution, and we compared them against the L_2-errors of stochastic collocation solutions obtained with $N_z = 2^n$ ($n \in \{1, 2, 3\}$) sample points in the random space.

We present first in Figs. 17, 18 the results of the L_2-errors (in a $\log_{10}$ scale) for the mean and standard deviation of the density at the different times $t = 1.25, 2.5, 5, 10$ picoseconds of the evolution problem.

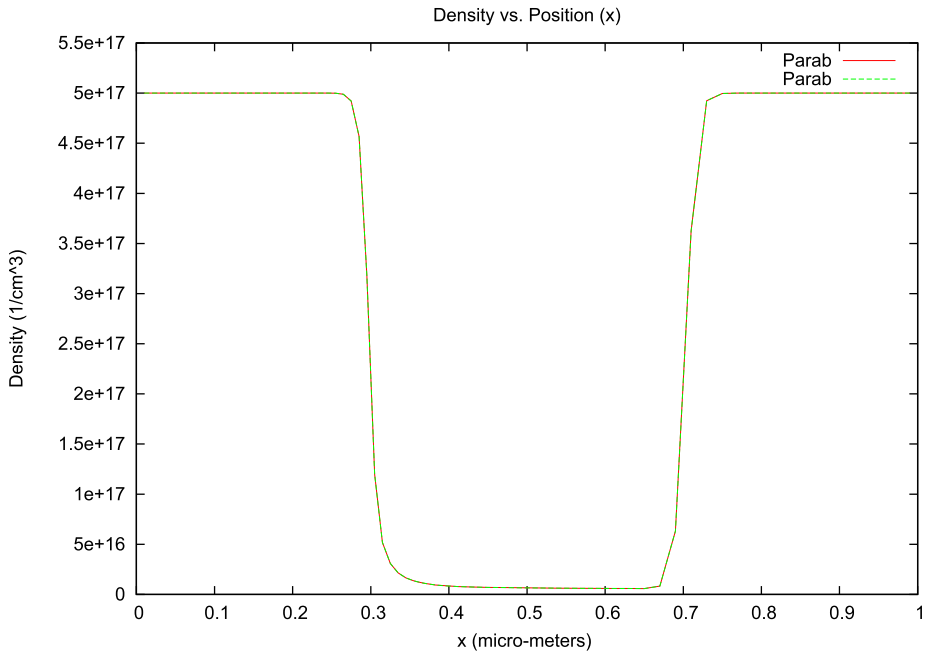

Fig. 9. Density $\rho(x, t_0)$ for a 1 µm diode, 0.5 V bias, and $t_0 = 10.0$ ps.

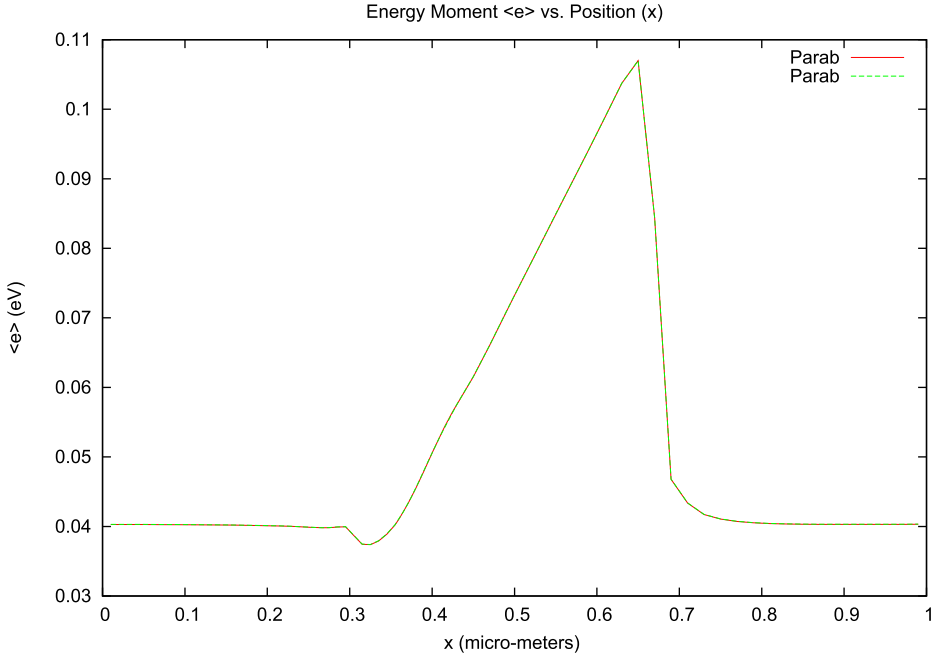

Fig. 10. Energy $e(x, t_0)$ for a 1 µm diode, 0.5 V bias, and $t_0 = 10.0$ ps.

The L_2-error of the density mean for our SG solution is higher than for the Stochastic Collocation solutions, which, except for a couple of points at the time $t = 1.25$ ps, have the expected ordering with respect to the number of sample points $N_z = 2, 4, 8$.

Likewise, the L_2-error for the density standard deviation of the SG solution is higher than for the SC solutions and slightly increases over time (corresponding to the behavior observed in Fig. 16). Again, except for two points at the initial time, the ordering of the SC solutions is the expected one given their number of sample points $N_z = 2, 4, 8$.

However, the density means and standard deviations only constitute quantities related to zeroth-order moments of the actual PDF where the random variable z has already been integrated for obtaining them before the calculation of the

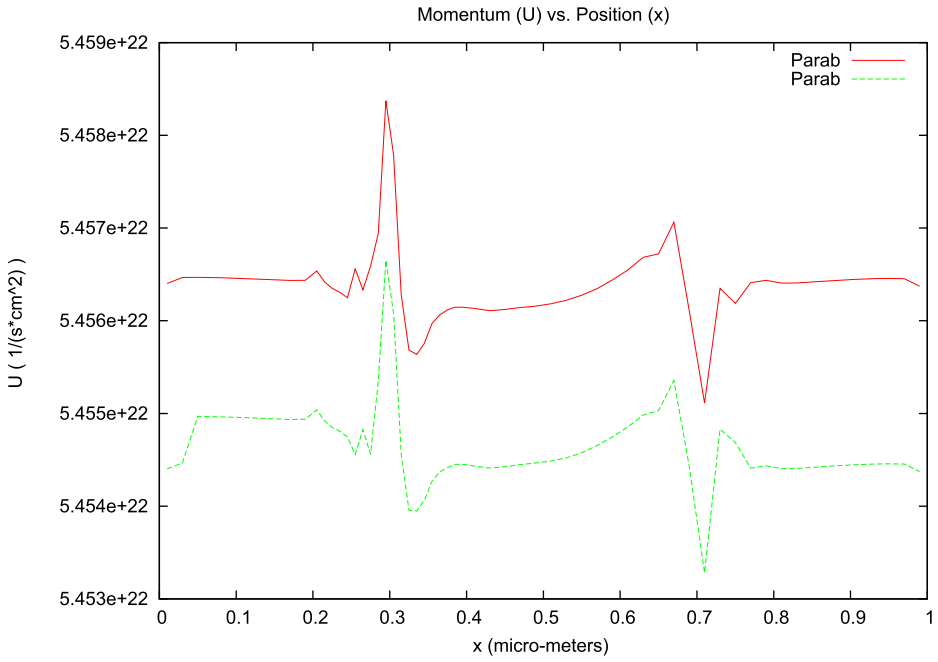

Fig. 11. Momentum (current) $M(x, t_0)$ for a 1 µm diode, 0.5 V bias, and $t_0 = 10.0$ ps.

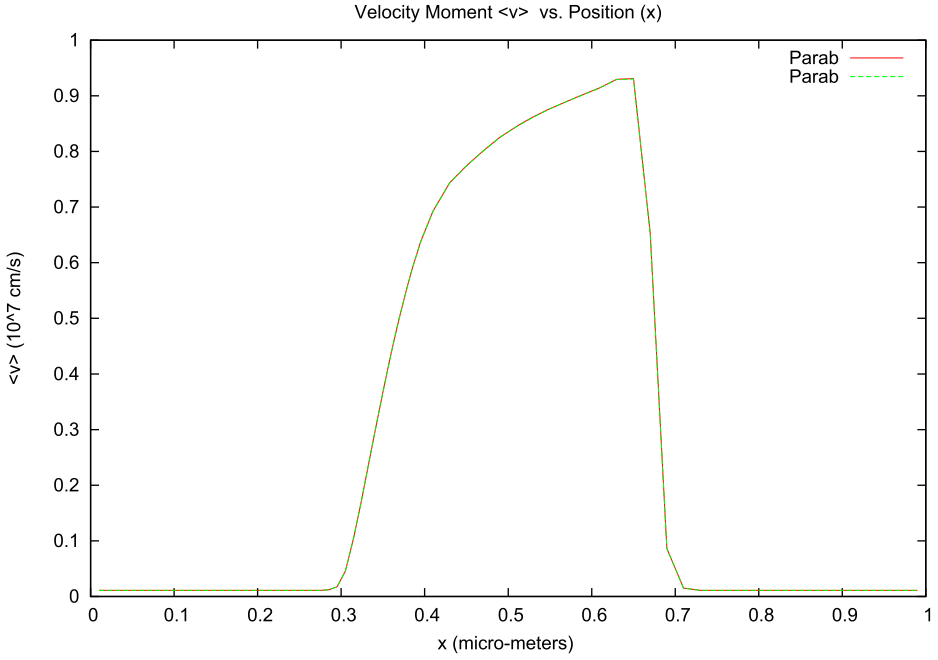

Fig. 12. Velocity $v(x, t_0)$ for a 1 µm diode, 0.5 V bias, and $t_0 = 10.0$ ps.

L_2-error. We consider then the L_2-errors of the transformed PDF $\Phi = \sqrt{r} f/2$ at the final time $t_f = 10$ ps of the evolution problem (where we will also have to integrate numerically over z during the needed computation to obtain these quantities), comparing the L_2-error of our stochastic Galerkin numerical solution w.r.t. the HO-SC against the L_2-errors of numerical solutions obtained via stochastic collocation with a number of samples $N_z = 2^n$, $n \in \{1, 2\}$. Fig. 19 shows that the L_2-error (in $\log_{10}$-scale) of our SG solution is below the respective one for the SC solutions, which decreases from $N_z = 2$ to $N_z = 4$. We then have that the error of our SG solution is slightly below the respective one for $N_z = 4$ and therefore our SG solution is slightly closer to the HO-SC reference solution in the L_2-sense than a SC solution with $N_z = 4$.

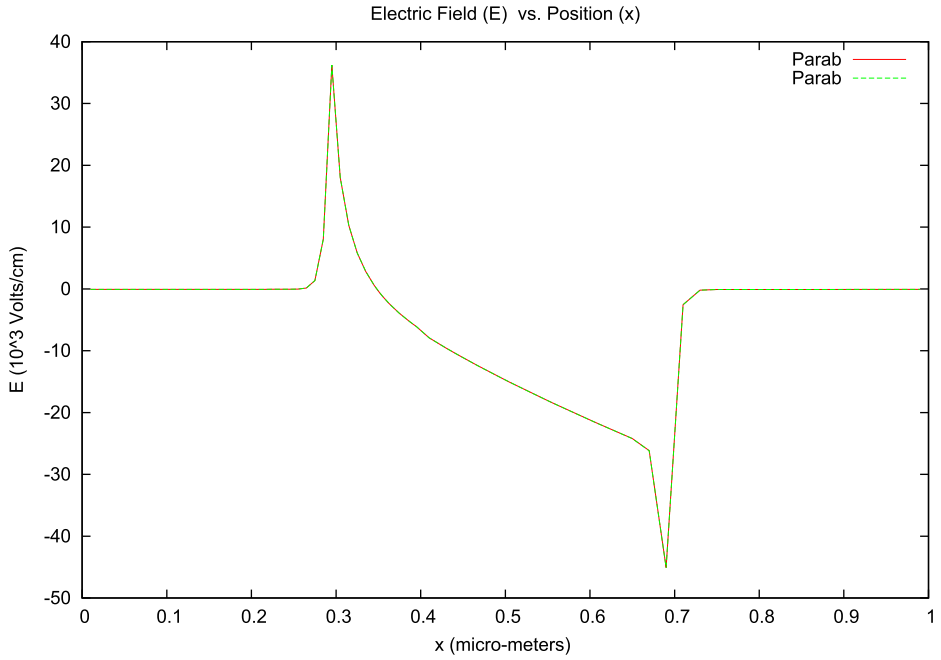

Fig. 13. Electric field $\mathrm{E}(x, t_0)$ for a 1 µm diode, 0.5 V bias, and $t_0 = 10.0$ ps.

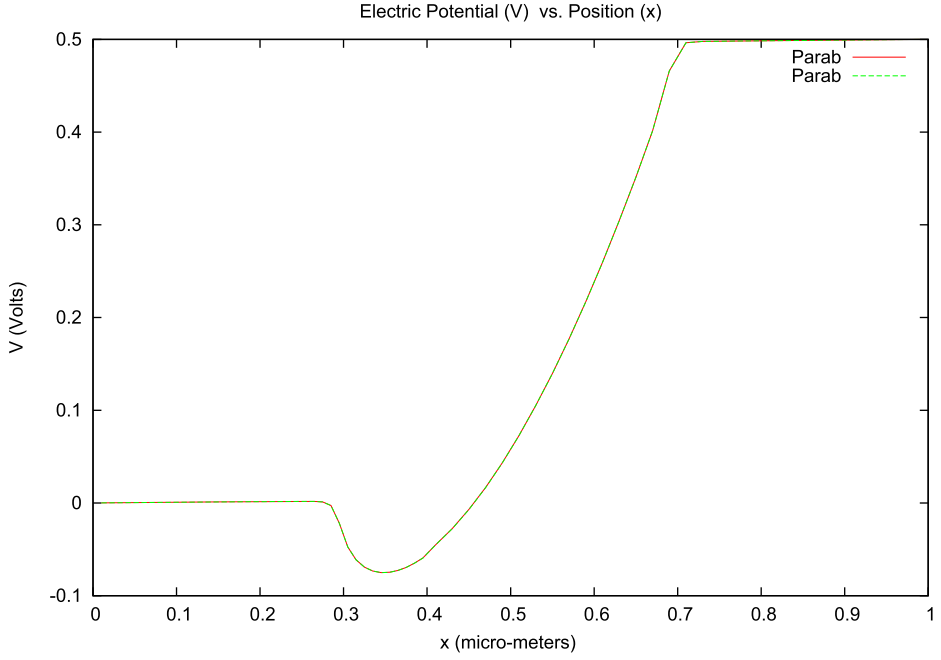

Fig. 14. Potential $V(x, t_0)$ for a 1 µm diode, 0.5 V bias, and $t_0 = 10.0$ ps.

5. Sensitivity analysis & stability of a sG-DG scheme

5.1. Randomness in initial condition under an entropy norm with periodic BC

We will derive a sensitivity analysis result for the case of randomness in the initial condition of our problem, when a semi-discrete DG scheme for the sG numerics works under an entropy norm, under periodic boundary conditions. This result in 1D position space is a simpler version of a similar result for 2D position space, to appear in [29], that considers randomness in the initial condition and the problem being under both periodic and specular boundary conditions, which is

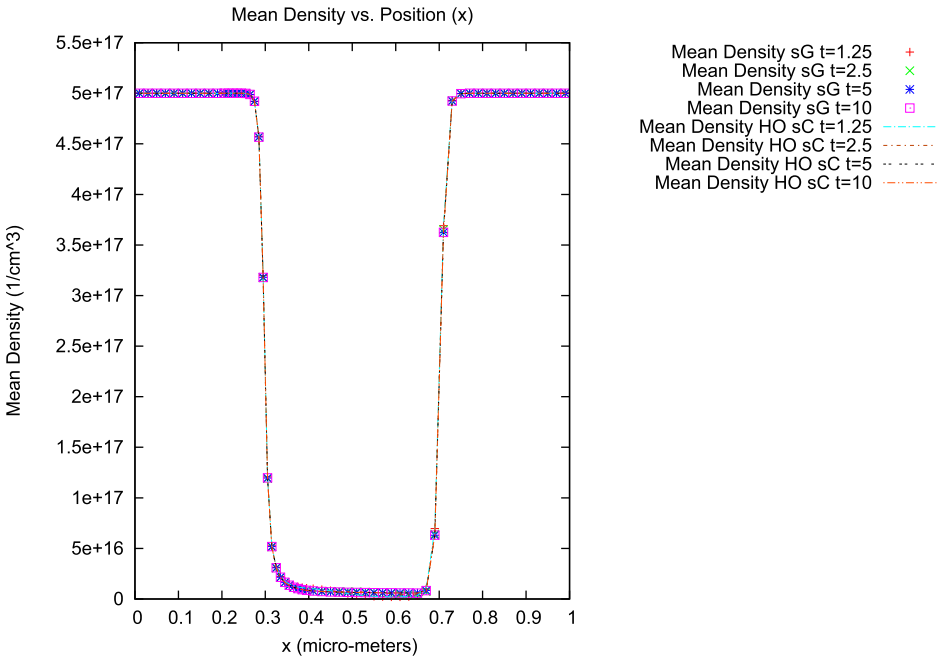

Fig. 15. Mean density $\rho(x,t)$ for both the stochastic Galerkin (sG) and the high-order stochastic collocation (HO-SC) solutions at the different times $t = 1.25, 2.5, 5, 10$ picoseconds of our evolution problem.

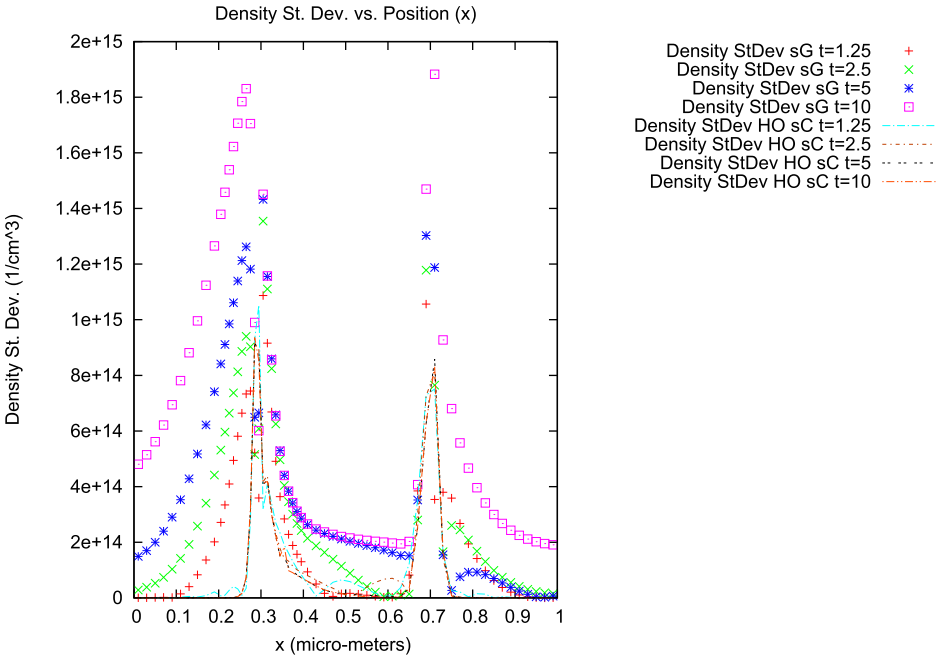

Fig. 16. Density Standard Deviation for both the stochastic Galerkin (sG) and the high-order stochastic collocation (HO-SC) solutions at the different times $t = 1.25, 2.5, 5, 10$ picoseconds of our evolution problem.

itself inspired on the deterministic result for entropy-stable positivity-preserving DG schemes found in [30] that considers both periodic and specular boundary conditions for 2D devices.

If we consider the norm below frequently used in uncertainty quantification analysis,

$$\|f\|_{H_z^\kappa} = \sqrt{\sum_{k=0}^{\kappa} ||\partial_z^k f||_{L_z^2}^2} \tag{43}$$

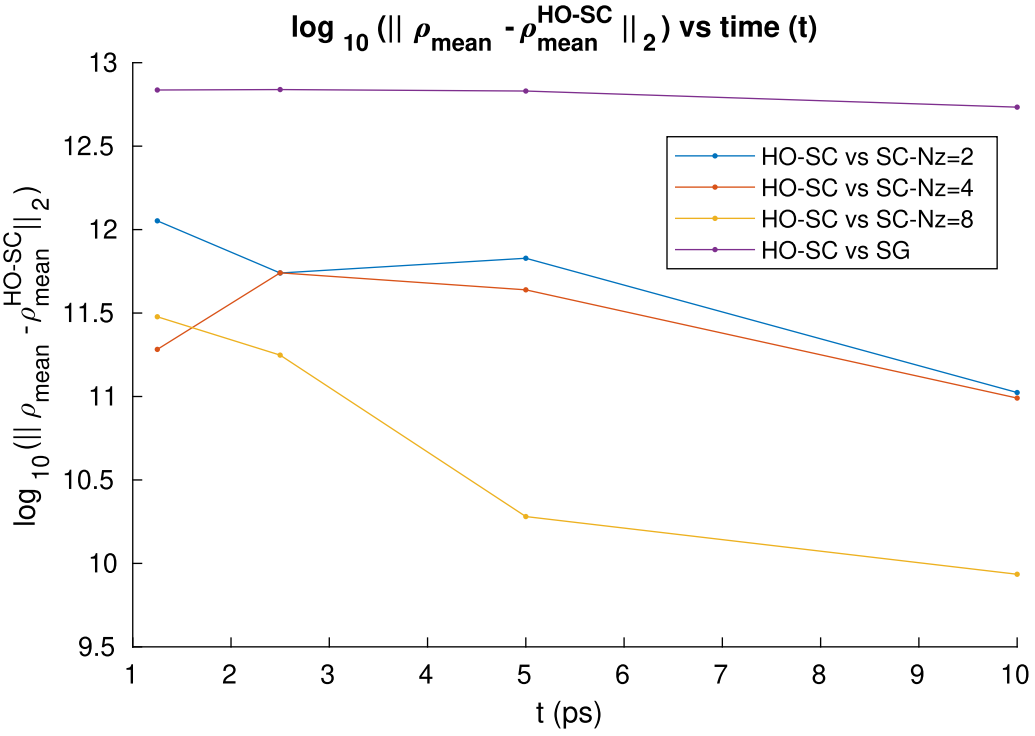

Fig. 17. Mean density L_2 error in $\log_{10}$-scale for our SG solution and for SC solutions with $N_z = 2^n$, $n \in \{1, 2, 3\}$ sample points, at the different times $t = 1.25, 2.5, 5, 10.0$ ps.

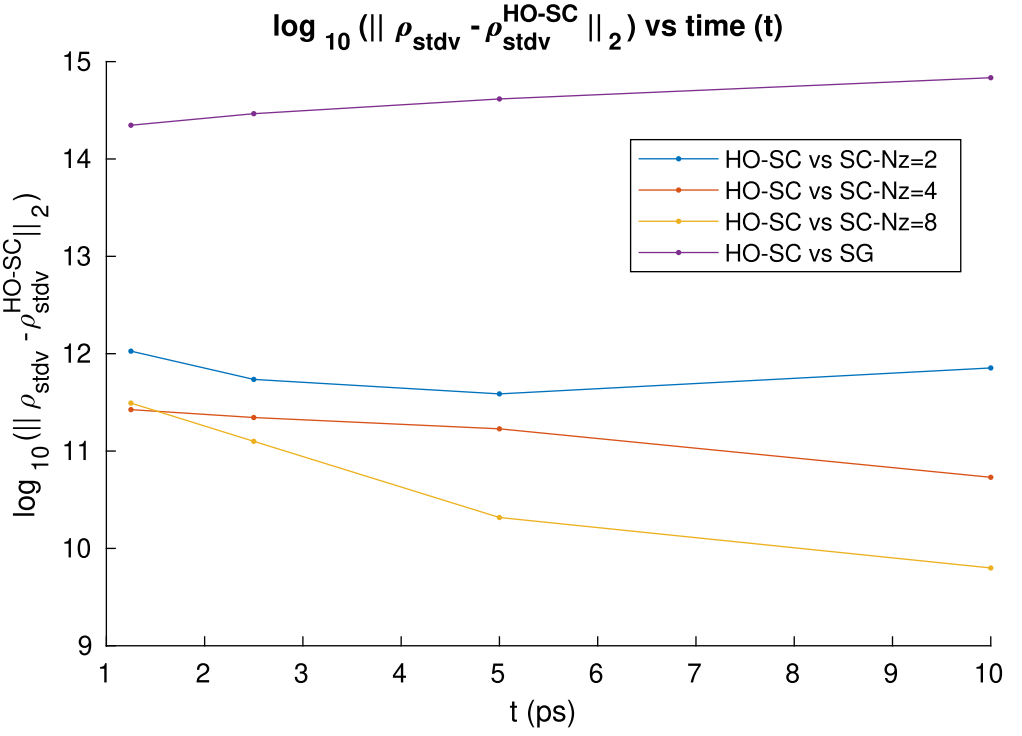

Fig. 18. L_2 error (in $\log_{10}$-scale) of the density standard deviation for our SG solution and for SC solutions with $N_z = 2^n$, $n \in \{1, 2, 3\}$ sample points, at the different times $t = 1.25, 2.5, 5, 10.0$ ps.

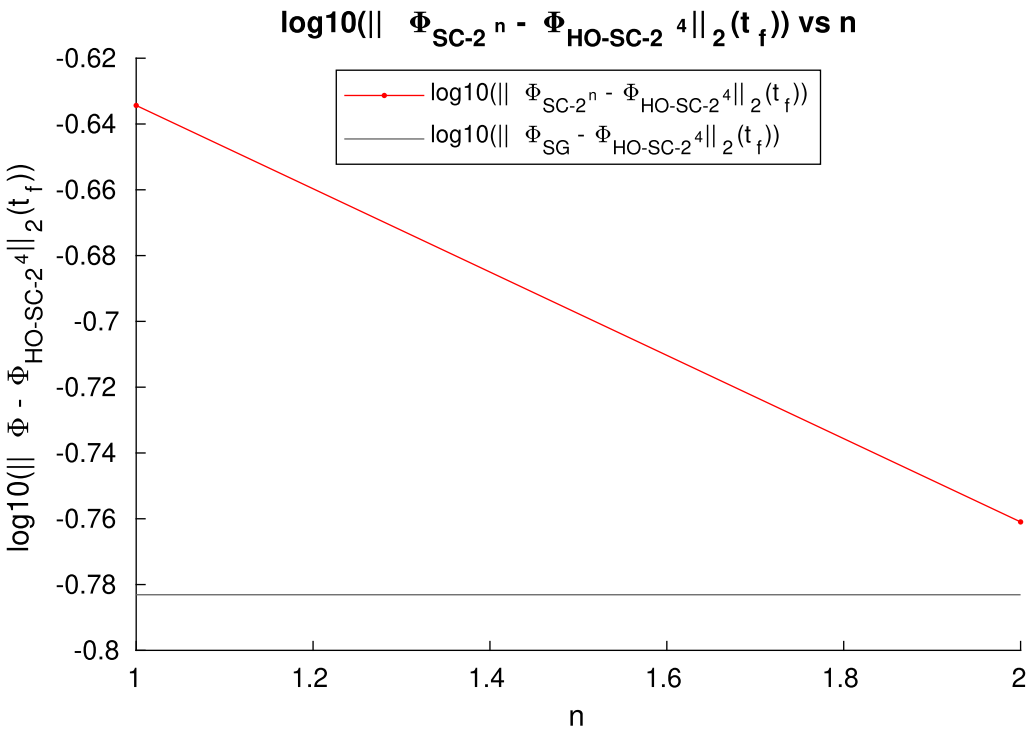

Fig. 19. L_2 error (in $\log_{10}$-scale) of the transformed PDF $\Phi = \sqrt{r} f/2$ at the final time $t_f = 10$ ps for our SG solution and for SC solutions with $N_z = 2^n$ ($n \in 1, 2$) sample points versus $n = \log_2(N_z)$.

based on the following L_z^2-norm in the random space I_z,

$$\|f\|_{L_z^2} = \sqrt{\int_{I_z} \pi(z) |f|^2 dz}, \tag{44}$$

we have that, if the initial condition f_0 of our semi-discrete scheme has a finite H_z^κ-norm, then the z-derivatives up to order κ of f_h, namely $\partial_z^k f_h$ with $0 \leq k \leq \kappa$, are stable under an entropy norm in the following sense,

$$0 \geq \frac{1}{2} \int_\Omega \partial_t (\partial_z^k f_h)^2 \exp(H) d\vec{x} d\vec{k} \tag{45}$$

when periodic boundary conditions in $\vec{x}$ are assumed for the problem and also that the electric field is a given known function $\vec{E}(\vec{x}, t)$.

We prove the claim above as follows. Taking a k-th order z-derivative over our Boltzmann equation, we have

$$\partial_t (\partial_z^k f_h) + \frac{1}{\hbar} \nabla_{\vec{k}} \varepsilon(\vec{k}) \cdot \nabla_{\vec{x}} (\partial_z^k f_h) - \frac{q}{\hbar} \vec{E}(\vec{x}, t) \cdot \nabla_{\vec{k}} (\partial_z^k f_h) = Q(\partial_z^k f_h), \tag{46}$$

since we have assumed the uncertainty appears only in the initial condition, and the collision term is a linear operator of f, even if it includes delta distributions in its scattering kernel.

We will use an entropy inequality that our Boltzmann equation for electrons in semiconductors satisfies, namely

$$0 \geq \int_\Omega Q(f) f \exp(H) d\vec{x} d\vec{k}. \tag{47}$$

This inequality applies to $\partial_z^k f_h$ as well. Plugging into this inequality $\partial_z^k f_h$ then, we have

$$0 \geq \int_\Omega Q(\partial_z^k f_h) \partial_z^k f_h \exp(H) d\vec{x} d\vec{k}, \tag{48}$$

which we will use relating it to the collisional term appearing in a DG scheme, under an entropy norm, where the weak form of the Boltzmann equation for the z-derivatives of f is expressed. Concretely, we have

$$0 \geq \int_{\Omega} Q\,(\partial_z^k f_h)\partial_z^k f_h e^H d\vec{x}d\vec{k} = \int_{\Omega} d\vec{k}d\vec{x}\partial_z^k f_h e^H \partial_t(\partial_z^k f_h) \tag{49}$$
$$+ \int_{\Omega} d\vec{k}d\vec{x}\partial_z^k f_h e^H \nabla_{\vec{x}} \cdot (\partial_z^k f_h \frac{1}{\hbar}\nabla_{\vec{k}}\,\varepsilon(\vec{k})) - \int_{\Omega} d\vec{k}d\vec{x}\partial_z^k f_h e^H \nabla_{\vec{k}} \cdot (\partial_z^k f_h \frac{q}{\hbar}\vec{E})$$

whose right hand side renders via integration by parts over the whole phase space domain the weak form of a DG scheme,

$$0 \geq \int_{\Omega} d\vec{k}d\vec{x}\partial_z^k f_h e^H \partial_t(\partial_z^k f_h) + \int_{\partial_{\vec{x}}\Omega} d\sigma\, \partial_z^k f_h e^H \widehat{\partial_z^k f_h} \frac{1}{\hbar}\nabla_{\vec{k}}\,\varepsilon(\vec{k}) \cdot \hat{n} \tag{50}$$
$$- \int_{\Omega} d\vec{k}d\vec{x}\partial_z^k f_h \frac{1}{\hbar}\nabla_{\vec{k}}\,\varepsilon(\vec{k}) \cdot \nabla_{\vec{x}}(\partial_z^k f_h e^H)$$
$$- \int_{\partial_{\vec{k}}\Omega} d\sigma\, \partial_z^k f_h e^H \widehat{\partial_z^k f_h} \frac{q}{\hbar}\vec{E} \cdot \hat{n} + \int_{\Omega} d\vec{k}d\vec{x}\nabla_{\vec{k}}(\partial_z^k f_h e^H) \cdot \partial_z^k f_h \frac{q}{\hbar}\vec{E},$$

making use of the numerical flux in the boundary integrals. If we now consider the transport vector $\frac{1}{\hbar}(\nabla_{\vec{k}}\,\varepsilon(\vec{k}), -q\vec{E})$, it is clear that

$$\nabla_{(\vec{x},\vec{k})} \cdot (\frac{\nabla_{\vec{k}}\varepsilon(\vec{k})}{\hbar}, \frac{-q\vec{E}(x,t)}{\hbar}) = 0$$

holds, and it is also known, due to the Hamiltonian nature of the transport terms, that

$$\frac{1}{\hbar}(\nabla_{\vec{k}}\,\varepsilon(\vec{k}), -q\vec{E}) \cdot \nabla_{(\vec{x},\vec{k})} H = 0. \tag{51}$$

It can be proven that our transport integrals satisfy the following equation useful for the DG analysis,

$$\int_{\Omega} d\vec{x}d\vec{k}\partial_z^k f_h \frac{(\nabla_{\vec{k}}\,\varepsilon(\vec{k}), -q\vec{E})}{\hbar} \cdot \nabla_{(\vec{x},\vec{k})}(\partial_z^k f_h e^H) = \frac{\int_{\partial\Omega} d\sigma\, \partial_z^k f_h (\nabla_{\vec{k}}\,\varepsilon(\vec{k}), -q\vec{E}) \cdot \hat{n}\partial_z^k f_h e^H}{2\hbar}$$

where the transport in both $\vec{x}$, $\vec{k}$-boundaries of the phase space is expressed abbreviated jointly. The proof relies on integration by parts and on the divergence-free nature of the transport field in the phase space. Inserting this relation into the entropy inequality of our DG scheme, we have

$$0 \geq \int_{\Omega} d\vec{k}d\vec{x}\partial_z^k f_h e^H \partial_t(\partial_z^k f_h)$$
$$+ \int_{\partial_{\vec{x}}\Omega} d\sigma\, \partial_z^k f_h e^H \widehat{\partial_z^k f_h} \frac{1}{\hbar}\nabla_{\vec{k}}\,\varepsilon(\vec{k}) \cdot \hat{n} - \frac{1}{2}\int_{\partial_{\vec{x}}\Omega} d\sigma\, \partial_z^k f_h e^H \partial_z^k f_h \frac{1}{\hbar}\nabla_{\vec{k}}\,\varepsilon(\vec{k}) \cdot \hat{n}$$
$$- \int_{\partial_{\vec{k}}\Omega} d\sigma\, \partial_z^k f_h e^H \widehat{\partial_z^k f_h} \frac{q}{\hbar}\vec{E} \cdot \hat{n} + \frac{1}{2}\int_{\partial_{\vec{k}}\Omega} d\sigma\, \partial_z^k f_h e^H \partial_z^k f_h \frac{q}{\hbar}\vec{E} \cdot \hat{n}.$$

We can consider the integration over all the domain as an integration over the union of the whole set of elements in the DG FEM scheme. We will now pair together then, for two neighboring elements, their respective overlapping edges, for which it holds that $\hat{n}_1 = -\hat{n}_2$ and the transport vector has the same value over them. Then, we divide the edges between the internal ones and the associated to external boundaries. The edges related to the boundary have either periodic (in $\vec{x}$) or cut-off (in $\vec{k}$) boundary conditions applied over them. Therefore we only need to consider the $\vec{x}$-boundary integrals since the $\vec{k}$-boundary integrals will vanish. We can then simply distinguish between internal edges (IE) and boundary edges with periodic BC in $\vec{x}$ (PB) when we consider the integrals over all edges, that is, $\partial\Omega = IE \cup PB$, and

$$0 \geq \int_{\Omega} d\vec{k}d\vec{x}\partial_z^k f_h e^H \partial_t(\partial_z^k f_h) + \int_{\partial\Omega} d\sigma\, \partial_z^k f_h e^H \widehat{\partial_z^k f_h} \frac{(\nabla_{\vec{k}}\varepsilon(\vec{k}), -q\vec{E})}{\hbar} \cdot \hat{n}$$
$$- \frac{1}{2}\int_{\partial\Omega} d\sigma\, \partial_z^k f_h e^H \partial_z^k f_h \frac{(\nabla_{\vec{k}}\varepsilon(\vec{k}), -q\vec{E})}{\hbar} \cdot \hat{n}.$$

The periodic boundaries can be handled in a similar fashion to internal edges, since for both of them the conditions over edge pairs $\hat{n}_1 = -\hat{n}_2$ and equal value of the transport vector over them hold. We then proceed to divide within edges between inflow regions, for which $(\nabla_{\vec{k}}\varepsilon(\vec{k}), -q\vec{E}) \cdot \hat{n} < 0$, and outflow regions over which $(\nabla_{\vec{k}}\varepsilon(\vec{k}), -q\vec{E}) \cdot \hat{n} > 0$. This is done to compare the value of the test function over a boundary to the numerical flux value $\widehat{\partial_z^k f_h} = (\partial_z^k f_h)^-$ according to the upwind rule. The test function value over outflow boundaries is $(\partial_z^k f_h)^-$, and over inflow boundaries is $(\partial_z^k f_h)^+$. Therefore we have that

$$
\begin{aligned}
0 \geq & \int_\Omega d\vec{k}d\vec{x}\partial_z^k f_h e^H \partial_t(\partial_z^k f_h) \\
& + \int_{(\nabla_{\vec{k}}\varepsilon, -q\vec{E})\cdot\hat{n}<0} d\sigma\, \partial_z^k f_h e^H \widehat{\partial_z^k f_h} \frac{(\nabla_{\vec{k}}\varepsilon(\vec{k}), -q\vec{E})}{\hbar} \cdot \hat{n} \\
& + \int_{(\nabla_{\vec{k}}\varepsilon, -q\vec{E})\cdot\hat{n}>0} d\sigma\, \partial_z^k f_h e^H \widehat{\partial_z^k f_h} \frac{(\nabla_{\vec{k}}\varepsilon(\vec{k}), -q\vec{E})}{\hbar} \cdot \hat{n} \\
& - \frac{1}{2} \int_{(\nabla_{\vec{k}}\varepsilon, -q\vec{E})\cdot\hat{n}<0} d\sigma\, \partial_z^k f_h e^H \partial_z^k f_h \frac{(\nabla_{\vec{k}}\varepsilon(\vec{k}), -q\vec{E})}{\hbar} \cdot \hat{n} \\
& - \frac{1}{2} \int_{(\nabla_{\vec{k}}\varepsilon, -q\vec{E})\cdot\hat{n}>0} d\sigma\, \partial_z^k f_h e^H \partial_z^k f_h \frac{(\nabla_{\vec{k}}\varepsilon(\vec{k}), -q\vec{E})}{\hbar} \cdot \hat{n}
\end{aligned} \tag{52}
$$

is equal to

$$
\begin{aligned}
0 \geq & \int_\Omega d\vec{k}d\vec{x}\partial_z^k f_h e^H \partial_t(\partial_z^k f_h) \\
& + \int_{(\nabla_{\vec{k}}\varepsilon, -q\vec{E})\cdot\hat{n}<0} d\sigma\, (\partial_z^k f_h)^+ e^H (\partial_z^k f_h)^- \frac{(\nabla_{\vec{k}}\varepsilon(\vec{k}), -q\vec{E})}{\hbar} \cdot \hat{n} \\
& + \int_{(\nabla_{\vec{k}}\varepsilon, -q\vec{E})\cdot\hat{n}>0} d\sigma\, (\partial_z^k f_h)^- e^H (\partial_z^k f_h)^- \frac{(\nabla_{\vec{k}}\varepsilon(\vec{k}), -q\vec{E})}{\hbar} \cdot \hat{n} \\
& - \frac{1}{2} \int_{(\nabla_{\vec{k}}\varepsilon, -q\vec{E})\cdot\hat{n}<0} d\sigma\, (\partial_z^k f_h)^+ e^H (\partial_z^k f_h)^+ \frac{(\nabla_{\vec{k}}\varepsilon(\vec{k}), -q\vec{E})}{\hbar} \cdot \hat{n} \\
& - \frac{1}{2} \int_{(\nabla_{\vec{k}}\varepsilon, -q\vec{E})\cdot\hat{n}>0} d\sigma\, (\partial_z^k f_h)^- e^H (\partial_z^k f_h)^- \frac{(\nabla_{\vec{k}}\varepsilon(\vec{k}), -q\vec{E})}{\hbar} \cdot \hat{n}.
\end{aligned} \tag{53}
$$

If we simplify this expression we get

$$
\begin{aligned}
0 \geq & \int_\Omega d\vec{k}d\vec{x}\partial_z^k f_h e^H \partial_t(\partial_z^k f_h) \\
& - \int_{(\nabla_{\vec{k}}\varepsilon, -q\vec{E})\cdot\hat{n}<0} d\sigma\, (\partial_z^k f_h)^+ e^H (\partial_z^k f_h)^- \frac{|(\nabla_{\vec{k}}\varepsilon(\vec{k}), -q\vec{E}) \cdot \hat{n}|}{\hbar} \\
& + \frac{1}{2} \int_{(\nabla_{\vec{k}}\varepsilon, -q\vec{E})\cdot\hat{n}>0} d\sigma\, (\partial_z^k f_h)^- e^H (\partial_z^k f_h)^- \frac{|(\nabla_{\vec{k}}\varepsilon(\vec{k}), -q\vec{E}) \cdot \hat{n}|}{\hbar}
\end{aligned}
$$

$$+\frac{1}{2}\int\limits_{(\nabla_{\vec{k}}\varepsilon,-q\vec{E})\cdot\hat{n}<0} d\sigma\,(\partial_z^k f_h)^+ e^H (\partial_z^k f_h)^+ \frac{|(\nabla_{\vec{k}}\varepsilon(\vec{k}),-q\vec{E})\cdot\hat{n}|}{\hbar} \tag{54}$$

or equivalently

$$\begin{aligned}
0 \geq & \int\limits_{\Omega} d\vec{k}d\vec{x}\partial_z^k f_h e^H \partial_t(\partial_z^k f_h) \\
& + \frac{1}{2}\left(\int\limits_{(\nabla_{\vec{k}}\varepsilon,-q\vec{E})\cdot\hat{n}>0} d\sigma\,(\partial_z^k f_h)^- e^H (\partial_z^k f_h)^- \frac{|(\nabla_{\vec{k}}\varepsilon(\vec{k}),-q\vec{E})\cdot\hat{n}|}{\hbar} \right. \\
& - 2\int\limits_{(\nabla_{\vec{k}}\varepsilon,-q\vec{E})\cdot\hat{n}<0} d\sigma\,(\partial_z^k f_h)^+ e^H (\partial_z^k f_h)^- \frac{|(\nabla_{\vec{k}}\varepsilon(\vec{k}),-q\vec{E})\cdot\hat{n}|}{\hbar} \\
& \left. + \int\limits_{(\nabla_{\vec{k}}\varepsilon,-q\vec{E})\cdot\hat{n}<0} d\sigma\,(\partial_z^k f_h)^+ e^H (\partial_z^k f_h)^+ \frac{|(\nabla_{\vec{k}}\varepsilon(\vec{k}),-q\vec{E})\cdot\hat{n}|}{\hbar} \right).
\end{aligned} \tag{55}$$

On the other hand, if we use a notation e_h for the edges that allows redundancy (meaning it allows to count the same edge twice, once for each cell to which it belongs), internal edges and boundary edges associated to our $\vec{x}$-periodic BC will be treated the same way, and under this notation (with a factor of 1/2 to balance the redundancy in counting in this edge notation), we have

$$\begin{aligned}
0 \geq & \int\limits_{\Omega} d\vec{k}d\vec{x}\partial_z^k f_h e^H \partial_t(\partial_z^k f_h) \\
& + \frac{1}{2}\cdot\frac{1}{2}\left(\int\limits_{e_h} d\sigma\,(\partial_z^k f_h)^- e^H (\partial_z^k f_h)^- \frac{|(\nabla_{\vec{k}}\varepsilon(\vec{k}),-q\vec{E})\cdot\hat{n}|}{\hbar} \right. \\
& - 2\int\limits_{e_h} d\sigma\,(\partial_z^k f_h)^+ e^H (\partial_z^k f_h)^- \frac{|(\nabla_{\vec{k}}\varepsilon(\vec{k}),-q\vec{E})\cdot\hat{n}|}{\hbar} \\
& \left. + \int\limits_{e_h} d\sigma\,(\partial_z^k f_h)^+ e^H (\partial_z^k f_h)^+ \frac{|(\nabla_{\vec{k}}\varepsilon(\vec{k}),-q\vec{E})\cdot\hat{n}|}{\hbar} \right),
\end{aligned} \tag{56}$$

which is simply equal to

$$\begin{aligned}
0 \geq & \int\limits_{\Omega} d\vec{k}d\vec{x}\partial_z^k f_h e^H \partial_t(\partial_z^k f_h) \\
& + \frac{1}{4}\left(\int\limits_{e_h} d\sigma[(\partial_z^k f_h)^- + (\partial_z^k f_h)^+]^2 e^H \frac{|(\nabla_{\vec{k}}\varepsilon(\vec{k}),-q\vec{E})\cdot\hat{n}|}{\hbar} \right),
\end{aligned} \tag{57}$$

and, since the last term is non-negative, then

$$\begin{aligned}
0 &\geq -\frac{1}{4}\left(\int\limits_{e_h} d\sigma[(\partial_z^k f_h)^- + (\partial_z^k f_h)^+]^2 e^H \frac{|(\nabla_{\vec{k}}\varepsilon(\vec{k}),-q\vec{E})\cdot\hat{n}|}{\hbar} \right) \\
&\geq \int\limits_{\Omega} d\vec{k}d\vec{x}\partial_z^k f_h e^H \partial_t(\partial_z^k f_h) = \frac{1}{2}\int\limits_{\Omega} d\vec{k}d\vec{x} e^H \partial_t([\partial_z^k f_h]^2).
\end{aligned}$$

This is our stability result for the z-partials of f_h up to order κ for a DG scheme under an entropy norm. In the particular case that $\partial_t H = 0$, meaning for time-independent electric potentials, then this result implies that $0 \geq \partial_t \int_\Omega (\partial_z^k f_h)^2 e^H d\vec{k}d\vec{x}$.

5.2. Considerations on the bounds for the collision kernel related to randomness in the energy band

We now study the boundedness of the collision kernel for our problem in relation to possible randomness in the energy band, presenting a simplified case. We consider the Boltzmann equation for electrons in semiconductors assuming the electric field $E(x,t)$ is already known, and we will further assume that the uncertainty introduced in it, due to the coupling between the Boltzmann and the Poisson equation, is negligible.

If we make use of the Detailed Balance Principle known to hold for the Boltzmann-Poisson system, the linear collision operator can be written as

$$Q(f) = \int \sigma(k',k)[\frac{f'}{M'} - \frac{f}{M}]dk',$$

where

$$\sigma(k',k) = S(k',k)e^{-\frac{\varepsilon'}{K_B T_L}},$$

satisfying the symmetry condition

$$\sigma(k',k) = \sigma(k,k').$$

More explicitly,

$$\sigma(k',k) = e^{-\frac{\varepsilon'}{K_B T_L}}[K_0\delta(\varepsilon-\varepsilon') + Kn_q\{e^{\frac{\hbar\omega_p}{K_B T_L}}\delta(\varepsilon-\varepsilon'+\hbar\omega_p) + \delta(\varepsilon-\varepsilon'-\hbar\omega_p)\}],$$

therefore we equivalently have

$$Q(f) = \int [K_0\delta(\varepsilon-\varepsilon') + Kn_q\{e^{\frac{\hbar\omega_p}{K_B T_L}}\delta(\varepsilon-\varepsilon'+\hbar\omega_p) + \delta(\varepsilon-\varepsilon'-\hbar\omega_p)\}]M'[\frac{f'}{M'} - \frac{f}{M}]dk',$$

since $e^{-\frac{\varepsilon'}{K_B T_L}} = M'$, equivalent to

$$Q(f) = \int [K_0\delta(\varepsilon-\varepsilon') + Kn_q\{e^{\frac{\hbar\omega_p}{K_B T_L}}\delta(\varepsilon-\varepsilon'+\hbar\omega_p) + \delta(\varepsilon-\varepsilon'-\hbar\omega_p)\}]\frac{[Mf' - M'f]}{M}dk'.$$

We can use any of the forms above to study our collision operator when performing a coordinate transformation $k \to (\varepsilon, \mu, \varphi)$.

We have then

$$Q(f) = \int [K_0\delta(\varepsilon-\varepsilon') + Kn_q\{e^{\frac{\hbar\omega_p}{K_B T_L}}\delta(\varepsilon-\varepsilon'+\hbar\omega_p) + \delta(\varepsilon-\varepsilon'-\hbar\omega_p)\}][f' - (\frac{M'}{M})f]\frac{\partial k'}{\partial(\varepsilon',\mu',\varphi')}d\varepsilon' d\mu' d\varphi'$$

and if we simply denote $J' = \frac{\partial k'}{\partial(\varepsilon',\mu',\varphi')} = J(\varepsilon')$, under the assumption that this jacobian depends only on the energy (which is true when $\varepsilon(|\vec{k}|)$ holds), then

$$Q(f) = \int [K_0\delta(\varepsilon-\varepsilon') + Kn_q\{e^{\frac{\hbar\omega_p}{K_B T_L}}\delta(\varepsilon-\varepsilon'+\hbar\omega_p) + \delta(\varepsilon-\varepsilon'-\hbar\omega_p)\}][f' - (\frac{M'}{M})f]J'd\varepsilon' d\mu' d\varphi',$$

so splitting out the terms and applying the delta functionals (using afterwards a characteristic function χ over the energy variable),

$$\begin{aligned}
Q(f) &= K_0\int \delta(\varepsilon-\varepsilon')[f' - (\frac{M'}{M})f]J'd\varepsilon' d\mu' d\varphi' \\
&\quad + Kn_q\int e^{\frac{\hbar\omega_p}{K_B T_L}}\delta(\varepsilon-\varepsilon'+\hbar\omega_p)[f' - (\frac{M'}{M})f]J'd\varepsilon' d\mu' d\varphi' \\
&\quad + Kn_q\int \delta(\varepsilon-\varepsilon'-\hbar\omega_p)[f' - (\frac{M'}{M})f]J'd\varepsilon' d\mu' d\varphi', \qquad (58)\\
Q(f) &= K_0\int [f(\varepsilon,\mu',\varphi') - f]Jd\mu' d\varphi' + Kn_q\times \\
&\{\int e^{\frac{\hbar\omega_p}{K_B T_L}}[f(\varepsilon+\hbar\omega_p,\mu',\varphi') - M(\hbar\omega_p)f][J\chi](\varepsilon+\hbar\omega_p)d\mu' d\varphi' \\
&+ \int [f(\varepsilon-\hbar\omega_p,\mu',\varphi') - M(-\hbar\omega_p)f][J\chi](\varepsilon-\hbar\omega_p)d\mu' d\varphi'\},
\end{aligned}$$

$$Q(f) = K_0 \int [f(\varepsilon, \mu', \varphi') - f] J d\mu' d\varphi' +$$
$$Kn_q \{ \int [e^{\frac{\hbar\omega_p}{K_B T_L}} f(\varepsilon + \hbar\omega_p, \mu', \varphi') - f][J\chi](\varepsilon + \hbar\omega_p) d\mu' d\varphi'$$
$$+ \int [f(\varepsilon - \hbar\omega_p, \mu', \varphi') - e^{\frac{\hbar\omega_p}{K_B T_L}} f][J\chi](\varepsilon - \hbar\omega_p) d\mu' d\varphi' \}.$$

We can write then

$$Q(f) = \int K_0 [f(\varepsilon, \mu', \varphi') - f] J d\mu' d\varphi' +$$
$$\int Kn_q [(e^{\frac{\hbar\omega_p}{K_B T_L}})^{+1} f(\varepsilon + \hbar\omega_p, \mu', \varphi') - f][J\chi](\varepsilon + \hbar\omega_p) d\mu' d\varphi' +$$
$$\int Kn_q [f(\varepsilon - \hbar\omega_p, \mu', \varphi') - (e^{\frac{\hbar\omega_p}{K_B T_L}})^{+1} f][J\chi](\varepsilon - \hbar\omega_p) d\mu' d\varphi',$$

or

$$Q(f) = \int K_0 [f(\varepsilon, \mu', \varphi') - f] J d\mu' d\varphi'$$
$$+ \int Kn_q \sum_{0 \neq i = -1}^{+1} [(e^{\frac{\hbar\omega_p}{K_B T_L}})^{\frac{i+1}{2}} f(\varepsilon + i\hbar\omega_p, \mu', \varphi') - (e^{\frac{\hbar\omega_p}{K_B T_L}})^{\frac{1-i}{2}} f][J\chi](\varepsilon + i\hbar\omega_p) d\mu' d\varphi',$$

which is equivalent to

$$Q(f) = \int K_0 [f(\varepsilon, \mu', \varphi') - f] J d\mu' d\varphi'$$
$$+ \int Kn_q \sum_{\pm} [(e^{\frac{\hbar\omega_p}{K_B T_L}})^{\frac{1\pm1}{2}} f(\varepsilon \pm \hbar\omega_p, \mu', \varphi') - (e^{\frac{\hbar\omega_p}{K_B T_L}})^{\frac{1\mp1}{2}} f][J\chi](\varepsilon \pm \hbar\omega_p) d\mu' d\varphi'$$

or more succinctly

$$Q(f) = K_0 \int [f(\varepsilon, \mu', \varphi') - f] J d\mu' d\varphi' \tag{59}$$
$$+ Kn_q e^{\frac{\hbar\omega_p}{2K_B T_L}} \int \sum_{\pm} [e^{\frac{\pm\hbar\omega_p}{2K_B T_L}} f(\varepsilon \pm \hbar\omega_p, \mu', \varphi') - e^{\frac{\mp\hbar\omega_p}{2K_B T_L}} f][J\chi](\varepsilon \pm \hbar\omega_p) d\mu' d\varphi'.$$

Now we can indeed try to bound the collision scattering terms (both acoustic and optical) keeping in mind that $\varepsilon(k')$ acts as a sort of fixed parameter, and the integration is carried over (μ, φ) only. That is,

$$Q(f) = K_0 \int [f(\varepsilon, \mu', \varphi') - f] J d\mu' d\varphi' \tag{60}$$
$$+ \sum_{\pm} Kn_q e^{\frac{\hbar\omega_p}{2K_B T_L}} \int [e^{\frac{\pm\hbar\omega_p}{2K_B T_L}} f(\varepsilon \pm \hbar\omega_p, \mu', \varphi') - e^{\frac{\mp\hbar\omega_p}{2K_B T_L}} f][J\chi](\varepsilon \pm \hbar\omega_p) d\mu' d\varphi',$$

or

$$Q(f) = \sum_{i=-1}^{+1} K_i \int [e^{\frac{i\hbar\omega_p}{2K_B T_L}} f(\varepsilon + i\hbar\omega_p, \mu', \varphi') - e^{\frac{-i\hbar\omega_p}{2K_B T_L}} f][J\chi](\varepsilon + i\hbar\omega_p) d\mu' d\varphi',$$

with

$$K_1 = K_{-1} = Kn_q e^{\frac{\hbar\omega_p}{2K_B T_L}},$$

and since $n_q = (e^{\hbar\omega_p / K_B T_L} - 1)^{-1}$, then

$$K_{\pm 1} = K \frac{e^{\frac{\hbar\omega_p}{2K_B T_L}}}{e^{\hbar\omega_p / K_B T_L} - 1} = \frac{K}{e^{\frac{\hbar\omega_p}{2K_B T_L}} - e^{\frac{-\hbar\omega_p}{2K_B T_L}}} = \frac{K/2}{\sinh(\frac{\hbar\omega_p}{2K_B T_L})}.$$

Now we can bound the respective scattering kernels for each summand, up to a point. So we have

$$Q(f)(x,\varepsilon,\mu,\varphi)=\sum_{i=-1}^{+1}K_i\int_0^{2\pi}\int_{-1}^{+1}[J\chi](\varepsilon+i\hbar\omega_p)[\frac{f(\varepsilon+i\hbar\omega_p,\mu',\varphi')}{M(i\hbar\omega_p/2)}-M(\frac{i\hbar\omega_p}{2})f]d\mu'd\varphi'$$

since $M(\varepsilon)=e^{-\frac{\varepsilon}{K_BT_L}}$, or equivalently

$$Q(f)(x,\varepsilon,\mu,\varphi)=\sum_{i=-1}^{+1}K_i\int_0^{2\pi}\int_{-1}^{+1}[J\chi](\varepsilon+i\hbar\omega_p)[\frac{f'|_{\varepsilon'=\varepsilon+i\hbar\omega_p}}{M(i\hbar\omega_p/2)}-M(\frac{i\hbar\omega_p}{2})f]d\mu'd\varphi'$$

which is equal to

$$Q(f)(x,\varepsilon,\mu,\varphi)=\sum_{i=-1}^{+1}K_i\int_0^{2\pi}\int_{-1}^{+1}\frac{[J\chi](\varepsilon+i\hbar\omega_p)}{M(i\hbar\omega_p/2)}[f'|_{\varepsilon'=\varepsilon+i\hbar\omega_p}-M(i\hbar\omega_p)f]d\mu'd\varphi'$$

or

$$Q(f)(x,\varepsilon,\mu,\varphi)=\sum_{i=-1}^{+1}K_i\int_0^{2\pi}\int_{-1}^{+1}[J\chi](\varepsilon+i\hbar\omega_p)M(\frac{i\hbar\omega_p}{2})[\frac{f'|_{\varepsilon'=\varepsilon+i\hbar\omega_p}}{M(i\hbar\omega_p)}-f]d\mu'd\varphi',$$

and since

$$\frac{M'}{M}|_{\varepsilon'=\varepsilon+i\hbar\omega_p}=\frac{e^{-\frac{\varepsilon'}{K_BT_L}}}{e^{-\frac{\varepsilon}{K_BT_L}}}|_{\varepsilon'=\varepsilon+i\hbar\omega_p}=e^{-\frac{i\hbar\omega_p}{K_BT_L}}=M(i\hbar\omega_p),$$

they are equivalent to

$$Q(f)(x,\varepsilon,\mu,\varphi)=\sum_{i=-1}^{+1}K_i\int_0^{2\pi}\int_{-1}^{+1}\frac{[J\chi](\varepsilon+i\hbar\omega_p)}{M(i\hbar\omega_p/2)}[f'|_{\varepsilon'=\varepsilon+i\hbar\omega_p}-f\frac{M'}{M}|_{\varepsilon'=\varepsilon+i\hbar\omega_p}]d\mu'd\varphi',$$

or

$$Q(f)(x,\varepsilon,\mu,\varphi)=\sum_{i=-1}^{+1}K_i\int_0^{2\pi}\int_{-1}^{+1}[J\chi](\varepsilon+i\hbar\omega_p)M(\frac{i\hbar\omega_p}{2})[\frac{Mf'}{M'}|_{\varepsilon'=\varepsilon+i\hbar\omega_p}-f]d\mu'd\varphi',$$

both equivalent to

$$Q(f)(x,\varepsilon,\mu,\varphi)=\sum_{i=-1}^{+1}K_i\int_0^{2\pi}\int_{-1}^{+1}[J\chi](\varepsilon+i\hbar\omega_p)[\frac{Mf'}{M'}|_{\varepsilon'=\varepsilon+i\hbar\omega_p}-\frac{M'f}{M}|_{\varepsilon'=\varepsilon+i\hbar\omega_p}]d\mu'd\varphi'.$$

We now have

$$Q(f)=\sum_{i=-1}^{+1}K_i\int[e^{\frac{i\hbar\omega_p}{2K_BT_L}}f'|_{\varepsilon'=\varepsilon+i\hbar\omega_p}-e^{\frac{-i\hbar\omega_p}{2K_BT_L}}f][J\chi](\varepsilon+i\hbar\omega_p)d\mu'd\varphi',$$

and if we want to put it in a more symmetric form, then we conclude that if we want to have

$$\sum_{i=-1}^{+1}K_ie^{\frac{i\hbar\omega_p}{2K_BT_L}}[J\chi](\varepsilon+i\hbar\omega_p)M'|_{\varepsilon'=\varepsilon+i\hbar\omega_p}=\sum_{i=-1}^{+1}K_ie^{\frac{-i\hbar\omega_p}{2K_BT_L}}[J\chi](\varepsilon+i\hbar\omega_p)M,$$

we need

$$M'|_{\varepsilon'=\varepsilon+i\hbar\omega_p}e^{\frac{i\hbar\omega_p}{2K_BT_L}}=Me^{\frac{-i\hbar\omega_p}{2K_BT_L}},$$

equivalent to

$$e^{\frac{-i\hbar\omega_p}{K_BT_L}}=\frac{M'|_{\varepsilon'=\varepsilon+i\hbar\omega_p}}{M(\varepsilon)}=e^{\frac{-i\hbar\omega_p}{K_BT_L}}$$

which we have just shown it holds. So now we have three equivalent collision kernels

$$\tilde{\sigma}_i(k',k)|_{\varepsilon'=\varepsilon+i\hbar\omega_p} = K_i e^{\frac{i\hbar\omega_p}{2K_BT_L}}[J\chi](\varepsilon+i\hbar\omega_p)M(\varepsilon+i\hbar\omega_p)$$
$$= K_i e^{\frac{-i\hbar\omega_p}{2K_BT_L}}[J\chi](\varepsilon+i\hbar\omega_p)M(\varepsilon) = \tilde{\sigma}_i(k',k)|_{\varepsilon'=\varepsilon+i\hbar\omega_p}, \tag{61}$$

where, instead of the unbounded Dirac deltas, a bounded collision kernel appears, with the difference that it doesn't involve the argument $\varepsilon' = \varepsilon(k')$, as it has been already integrated (equivalent to the Dirac delta being evaluated).

This equivalent form with a bounded function is more amenable to the usual treatment in SG for kinetic equations where assumptions for the boundedness of the collision kernel (and sometimes its derivatives too) are usually required theoretically. We would have then the operator

$$Q(f) = \int \sum_{i=-1}^{1} \left[\tilde{\sigma}_i(k',k)\left(\frac{f'|_{\varepsilon'=\varepsilon+i\hbar\omega_p}}{M'} - \frac{f}{M}\right)\right]\Bigg|_{\varepsilon'=\varepsilon+i\hbar\omega_p} d\mu' d\varphi'$$

with the slight difference that the energy has already been evaluated (the effect of a Dirac delta functional) rather than appearing as the usual integration of a function over the energy variable. We have then equivalent forms for the collision scattering kernel, for $i \in \{-1, 0, 1\}$,

$$\tilde{\sigma}_i(k',k) = K_i[J\chi](\varepsilon+i\hbar\omega_p)M\left(\varepsilon+\frac{i\hbar\omega_p}{2}\right) = K_i e^{-\frac{\varepsilon+i\hbar\omega_p/2}{K_BT_L}}[J\chi](\varepsilon+i\hbar\omega_p) = \tilde{\sigma}_i(k',k).$$

Having this equivalent form for our collision kernel, attempts to use previously known analysis results for the sensitivity & UQ analysis in kinetic equations could be made provided this equivalent form for the kernel satisfies the needed assumptions.

6. Conclusions

Uncertainty quantification in the Boltzmann-Poisson system is crucial by the own probabilistic nature of the problem due to the high number of particles involved and due to its quantum mechanical features. Studying randomness in the temperature is an important leading example, both for reasons stemming from the physical nature of the problem – as the environment temperature may fluctuate – as well as related to the mathematical aspects, since the temperature is a scalar random variable that introduces randomness in the collision term and more precisely in the coefficients multiplying the Dirac delta distributions appearing in the electron-phonon collisions by the Fermi golden rule.

Our numerical results for the stochastic Galerkin method for the Boltzmann-Poisson system, assuming a random temperature in an electron-phonon collision operator, show a coefficient α_1 related to randomness, whose variations are located in similar regions of the phase space to the ones of the average term α_0, which has no randomness but shows finer and more pronounced variations.

Our comparison of SDG-BP with recombination terms against the no-recombination case, using the mean term α_0 in both cases to calculate the moments, shows only a difference in the moment (current) between these two cases. We have to remember that the moment is the product of density and energy, which on their own scales do not seem to exhibit a large difference between these two cases. However, the moment has a value close to a constant over the position domain when equilibrium is reached, and the difference in this mean value is observed between the two cases, although it is two orders of magnitude below the average value of the current (Fig. 11). Here a truncated random expansion up to first order in z was employed, which therefore discards terms of order z^2 whose average is non-zero over the domain. This is the likely explanation for the slight difference in the momentum values between the random and deterministic simulations.

We have also devised numerical methods for quantifying uncertainty related to the phonon energy via stochastic Galerkin methods, which can be handled by the introduction of distributional derivatives with respect to the random variable. This mathematical structure departs from the usual form of the collision term in stochastic Galerkin for Boltzmann models by the need of distributional derivatives in the random space, being the first case in stochastic Galerkin methods for kinetic equations where this structure appears, and opening a new analytical treatment of randomness in the aforementioned stochastic method.

In conclusion, we have handled in this work the possible uncertainties arising in a model of electron transport in semiconductors by stochastic Galerkin, mainly related to the collision mechanisms in this paper. We calculate the propagated uncertainty in the electron probability density function due to possible uncertainties in either the phonon energy (adding a random variable given by either a Gaussian or uniform distribution, considering first an approximate randomness to first order in the phonon energy and then the full calculation) or in the lattice temperature (assumed to vary randomly according to a uniform distribution).

Our purpose is to observe how physical variables which can either behave randomly in a real world setting (such as a varying temperature) or are known to be described approximately in our model (such as the phonon energy, which is often assumed to be constant, but really is known experimentally to be not constant) can affect physical observables such as

electric current, average energy or density, since our kinetic model lets us calculate those measurable quantities by means of moments of the PDF.

Our study is useful to let us predict in real world settings the impact that uncertainties or limitations in commonly used idealized models have on the behavior of an electronic device such as a diode or a MOSFET. This study is also useful in terms of introducing uncertainties in the energy transition arguments of the collision integrals with the ultimate goal of jumping from the scalar treatment presented in this paper to the case of an energy band structure $\varepsilon(\vec{k})$, which is a scalar function of a vector variable, in future work.

We have calculated with our numerical methods the variation in kinetic moments (density, mean energy, current, etc.) associated with a physically reasonable temperature variation in the lattice environment. We have presented the algorithms to make an approximate (to first order) and exact calculation of the propagation of uncertainty of the phonon energy (bounding the error of a constant phonon energy by a uniform distribution) into the PDF which will give as well the associated uncertainty in the prediction of moments.

CRediT authorship contribution statement

José A. Morales Escalante: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Resources, Software, Validation, Visualization, Writing – original draft, Writing – review & editing. **Clemens Heitzinger:** Conceptualization, Funding acquisition, Project administration, Resources, Supervision, Writing – original draft, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A

Examples of distributions for random phonon energy using a distributional derivative approximation

If we assume the example $\pi(z) := \frac{e^{-\frac{z^2}{2}}}{\sqrt{2}}$, $\Psi_1 := 1$, and $\Psi_2 := 2z$, we obtain

$$
\begin{aligned}
B(\vec{p},\vec{p}') &= \sigma_0(\vec{p},\vec{p}')\delta_{ij} - M^{-1}K \times \\
&\quad \left\{ \left[1 + \frac{1}{e^{\hbar\omega_p}-1} \right] \partial_z \left[\begin{pmatrix} 1 & 2z \\ 2z & 4z^2 \end{pmatrix} \pi(z) z \right] \chi|_{z=-(\varepsilon-\varepsilon'+\hbar\omega_p)} \right. \\
&\quad + (e^{\hbar\omega_p}-1)^{-1} \partial_z \left[\begin{pmatrix} 1 & 2z \\ 2z & 4z^2 \end{pmatrix} \pi(z) z \right] \chi|_{z=+(\varepsilon-\varepsilon'-\hbar\omega_p)} \\
&\quad \left. + \frac{e^{\hbar\omega_p} \sum_{\pm} \delta(\varepsilon-\varepsilon' \pm \hbar\omega_p)}{(e^{\hbar\omega_p}-1)^2} \begin{pmatrix} 0 & 1/2 \\ 1/2 & 0 \end{pmatrix} \right\} \\
&= \sigma_0(\vec{p},\vec{p}')\mathcal{I} - M^{-1}K \times \\
&\quad \left\{ \frac{e^{\hbar\omega_p}}{e^{\hbar\omega_p}-1} \begin{pmatrix} 1-z^2 & 2z(2-z^2) \\ 2z(2-z^2) & 2z^2(3-z^2) \end{pmatrix} \pi \chi|_{z=-(\varepsilon-\varepsilon'+\hbar\omega_p)} \right. \\
&\quad + \frac{1}{e^{\hbar\omega_p}-1} \begin{pmatrix} 1-z^2 & 2z(2-z^2) \\ 2z(2-z^2) & 2z^2(3-z^2) \end{pmatrix} \pi \chi|_{z=+(\varepsilon-\varepsilon'-\hbar\omega_p)} \\
&\quad \left. + \frac{e^{\hbar\omega_p}}{(e^{\hbar\omega_p}-1)^2} \sum_{\pm} \delta(\varepsilon-\varepsilon' \pm \hbar\omega_p) \begin{pmatrix} 0 & 1/2 \\ 1/2 & 0 \end{pmatrix} \right\}, \\
Q(\alpha) &= \int_{\Omega_{\vec{p}}} B(\vec{p},\vec{p}') \left[M(\vec{p})\alpha(\vec{p}') - M(\vec{p}')\alpha(\vec{p}) \right] d\vec{p}'.
\end{aligned}
$$

One could use, as another example, a distribution with compact support such that the probability density of having $z < -\hbar\omega_p$ would be zero.

Examples of distributions for the random phonon energy problem without approximation in the random space

If we assume a uniform distribution $\pi(z) = N/2\beta$ for $z \in [-\beta/N, \beta/N]$ with $N > 1$, or equivalently $\pi(w) = 1/2$ by the scaling $w = Nz/\beta$ for $w \in [-1, 1]$, with the associated Legendre polynomials $\Psi_1 = 1$ and $\Psi_2(w) = w$, we obtain

$$B = M^{-1}(\vec{p})K_0\delta(\varepsilon - \varepsilon')I + \frac{\frac{K\chi(z)/2}{1-e^{-\beta(\hbar\omega_p+z)}}\begin{pmatrix} 1 & \frac{Nz}{\beta} \\ \frac{Nz}{\beta} & (\frac{Nz}{\beta})^2 \end{pmatrix}\Big|_{z=\varepsilon'-\varepsilon-\hbar\omega_p} + \frac{K\chi(z)/2}{e^{\beta(\hbar\omega_p+z)}-1}\begin{pmatrix} 1 & \frac{Nz}{\beta} \\ \frac{Nz}{\beta} & (\frac{Nz}{\beta})^2 \end{pmatrix}\Big|_{z=\varepsilon-\varepsilon'-\hbar\omega_p}}{M(\vec{p})},$$

$$Q(\alpha) = \int_{\Omega_{\vec{p}}} B(\vec{p}, \vec{p'})\left[M(\vec{p})\alpha(\vec{p'}) - M(\vec{p'})\alpha(\vec{p})\right]d\vec{p'}.$$

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