

Deterministic Full-Band Boltzmann Equation Solver for 2D Materials

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Abstract—We present a deterministic full-band solver of the semiclassical Boltzmann equation (BE) for 2D materials, extending a Godunov-type stabilization scheme beyond the effective-mass approximation (EMA) to arbitrary band structures. The band structure of MoS₂ is computed using the tight-binding method and discretized on a triangular k-grid aligned to equi-energy lines over the full first Brillouin zone, ensuring detailed balance at equilibrium. Optical and acoustic phonon scattering, surface optical phonon scattering for a SiO₂ interface, and Coulomb center scattering are included. Crucially, the Pauli exclusion principle is incorporated directly, which is particularly important in 2D materials due to their low density of states. The results reveal a pronounced velocity overshoot caused by intervalley transfer between the K and Q valleys. To demonstrate the potential of the deterministic approach, we investigate soft plasma modes in a symmetric double-gate MoS₂/SiO₂ structure, yielding a peak oscillation frequency of 2.1 GHz. Kroemer’s criterion is satisfied over a wide range of wave numbers, suggesting the potential for soft plasma modes in these 2D electron systems.

Index Terms—Boltzmann transport equation, 2D materials, Godunov’s scheme, soft plasma waves.

I. INTRODUCTION

Since scaling of silicon FinFET technology beyond the 5-nm technology node leads to short-channel effects, which significantly degrade device performance, researchers are intensively investigating novel materials such as 2D materials as potential transport layers to sustain Moore’s Law [1]. Their atomic thickness promises scaling beyond the limits of conventional 3D semiconductors, while simultaneously mitigating limitations like mobility degradation and quantum confinement. Among these, monolayer MoS₂ is particularly attractive for transistor channels because it combines a moderate low-field mobility with a large intrinsic bandgap (≈ 1.8 eV), enabling low off-state leakage and high on/off ratios [2]. The design of 2D material transistors and the interpretation of experimental data are currently hindered by the lack of reliable, predictive simulation tools. Existing approaches have significant limitations: Non-Equilibrium Green’s Function (NEGF) solvers become prohibitively time-consuming when all relevant scattering mechanisms are included (e.g. [3]),

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while the drift-diffusion model relies on approximations that are questionable at today’s strongly scaled channel lengths.

We present a deterministic full-band solver of the semiclassical Boltzmann equation for 2D materials that takes into account the Pauli principle, the most relevant scattering mechanisms, and full bands over the entire first Brillouin zone. Compared with the widely used Monte Carlo (MC) approach (e.g. [4]), deterministic solvers offer distinct advantages. In particular, the Pauli principle can be included directly, which requires stringent approximations in the MC approach but cannot be neglected in 2D materials, where the density of states is low [5]. Moreover, steady-state and spatiotemporal small-signal solutions can be directly calculated by the deterministic solver, while the latter is very challenging for the transient MC method.

II. SIMULATION APPROACH

Assuming translation invariance for one dimension of the 2D material, the BE takes the form

$$\frac{\partial f}{\partial t} - \frac{eE_x}{\hbar} \frac{\partial f}{\partial k_x} + v_x \frac{\partial f}{\partial x} = \mathcal{S}(f), \quad (1)$$

where $f(\mathbf{k}, x, t)$ is the electron distribution function, E_x the x-component of the electric field, t the time, $\mathbf{k}$ the wave vector, v_x the x-component of the group velocity, and $\mathcal{S}(f)$ the scattering integral. In this work, $\mathcal{S}(f)$ incorporates optical and acoustic phonon scattering, surface optical phonon scattering

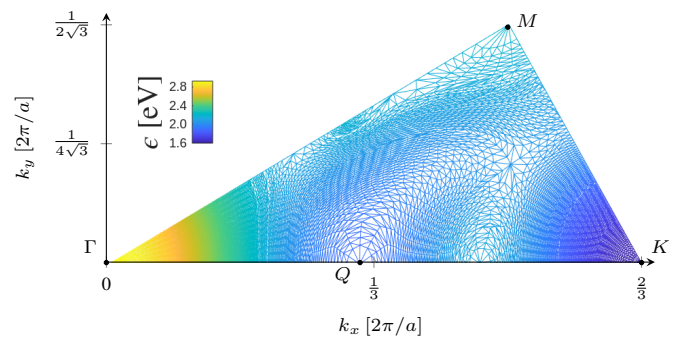


Fig. 1. Contour-aligned k-grid for the irreducible wedge of MoS₂ with a constant energy spacing of 5 meV.

(for SiO₂), and Coulomb center scattering with the scattering parameters from [4], while taking into account the Pauli exclusion principle. We compute the band structure using the tight-binding approach [6] and discretize the k-space with a triangular mesh aligned to equi-energy lines similar to [7] (Fig. 1). The contour alignment ensures that the principle of detailed balance is satisfied at equilibrium for the stabilization scheme used later [8]. The full-band description is crucial for 2D materials such as MoS₂, for which the (non-parabolic) effective-mass approximation (EMA) would introduce large errors in regions that contribute significantly to transport, because the valley minima K and Q lie close (Fig. 1).

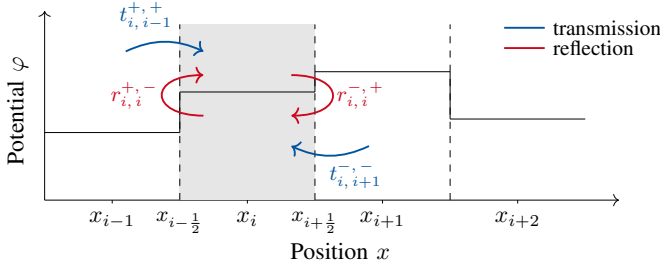


Fig. 2. Piecewise-constant potential profile used in the Godunov-type stabilization scheme. The grey region marks the Voronoi box $[x_{i-1/2}, x_{i+1/2}]$, where the transmission (blue) and reflection (red) are indicated for $v_x > 0$ (+) and $v_x < 0$ (-), respectively.

A. Godunov-type Stabilization Scheme

Solving the BE remains a numerically challenging task on today's computers [9]. We therefore build on the Godunov-type stabilization scheme, previously applied for III-V semiconductors with (non-parabolic) effective-mass approximation (EMA) [8], and extend it to full band structures. The first-order scheme ensures the nonnegativity of the distribution function regardless of the scattering mechanisms included, enabling numerically robust stationary, transient, and small-signal simulations [10]. Furthermore, we do not use the H-transformation but employ a fixed k-grid that is independent of the quasistatic potential (and thus time). This introduces numerical diffusion in k-space inherent to first-order upwinding, but its impact is small at room temperature [10] and it simplifies the implementation of transient and small-signal simulations.

The key idea is to move the problematic drift operator from the interior of each Voronoi box to the interfaces by assuming a piecewise-constant potential, which is illustrated in Fig. 2. As a result, E_x vanishes within each Voronoi box, separating the drift term from the other operators of Eq. (1). We use a piecewise-constant reconstruction of the distribution function

$$\bar{f}_i^j = \frac{1}{\Delta x_i} \frac{1}{\Omega_j} \int_{x_{i-1/2}}^{x_{i+1/2}} \iint_{\Gamma_j} f(\mathbf{k}, x, t) d^2\mathbf{k} dx \quad (2)$$

for each phase-space cell (i, j) , which refers to the j -th k-box (Γ_j) with area Ω_j and the i -th spatial Voronoi box. Integrating

over the finite volume of (i, j) then yields

$$\Omega_j \frac{\partial \bar{f}_i^j}{\partial t} + \frac{\mathcal{F}_{R,i}^j - \mathcal{F}_{L,i}^j}{\Delta x_i} = \mathcal{S}_i^j(\bar{f}). \quad (3)$$

The computation of fluxes at the left and right interfaces, $\mathcal{F}_{L,i}^j$ and $\mathcal{F}_{R,i}^j$, is nontrivial since the reconstruction of f is not continuous at the interfaces due to potential discontinuities. Godunov solved this issue by introducing a suitable Riemann solver that upwinds the fluxes according to the sign of the group velocity v_x^j in the transport direction [11], leading to:

$$\mathcal{F}_{L,i}^j = \begin{cases} \sum_{j'} t_{i,i-1}^{j,j'} \bar{f}_{i-1}^{j',+} + \sum_{m'} r_{i,i}^{j,m'} \bar{f}_i^{m',-} & \text{for } v_x^j > 0 \\ \Omega_j v_x^j \bar{f}_i^j & \text{for } v_x^j < 0 \end{cases} \quad (4)$$

and

$$\mathcal{F}_{R,i}^j = \begin{cases} \Omega_j v_x^j \bar{f}_i^j & \text{for } v_x^j > 0 \\ \sum_{j'} t_{i,i+1}^{j,j'} \bar{f}_{i+1}^{j',-} + \sum_{m'} r_{i,i}^{j,m'} \bar{f}_i^{m',+} & \text{for } v_x^j < 0 \end{cases} \quad (5)$$

Here, j' and m' denote transmission and reflection initial k-boxes, respectively; $(\cdot)^\pm$ indicates the sign of v_x for the corresponding initial k-box. The transmission coefficients $t_{i,i\pm 1}^{j,j'}$ and reflection coefficients $r_{i,i}^{j,m'}$ are calculated by the exact Riemann solver described in the next section.

When simulating a homogeneous 2D material, the spatial dependence is eliminated by assuming that the flux leaving the right boundary enters the left boundary for $v_x > 0$ and vice versa for $v_x < 0$. The BE is therefore solved for only one spatial cell and the electrostatic potential barrier is given by the product of $-E_x$ and the box width Δx_i . To impose a given electron density, the normalization condition

$$n = \frac{2}{(2\pi)^2} \iint_{\text{BZ}} f(\mathbf{k}, t) d^2\mathbf{k} \stackrel{!}{=} N_{2D} \quad (6)$$

replaces the BE of a single phase space cell, where N_{2D} is the electron density of the 2D electron gas.

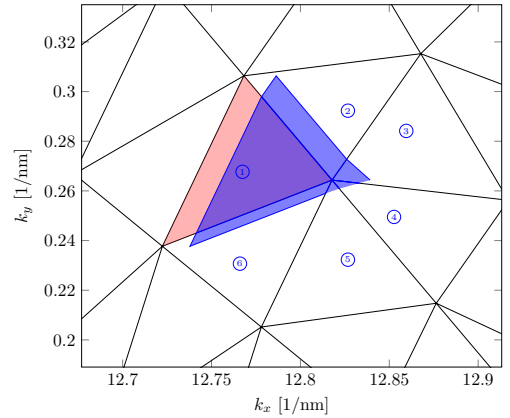


Fig. 3. Mapping of the final k-box (red) onto its initial k-boxes (blue) for the computation of the transmission and reflection coefficients. The blue polygons represent the portions of the initial k-boxes that contribute flux to the final k-box.

B. Riemann Solver for Full Bands

The transmission coefficients $t_{i,i\pm 1}^{j,j'}$ and reflection coefficients $r_{i,i}^{j,m'}$ are determined by the Riemann solver from the conservation conditions of flux, total energy, and the transverse wave vector component $k_{\parallel}$ (here: k_y). To this end, the band structure is decomposed into branches for a constant k_y value that are monotonically increasing or decreasing in energy along the transport direction x . Local extrema or saddle points lead to multiple branches, making the decomposition more complex than for monotonic bands (e.g. EMA). Nevertheless, the search for final states remains efficient using precomputed look-up tables on a fixed set of k_y values.

The backpropagation algorithm proceeds as follows. For a given final k-box j , the look-up tables for its k_y -range identify the candidate initial k-boxes from which flux may originate, accounting for the sign of Δk_x imposed by Newton's equation of motion $\hbar \frac{\partial k_x}{\partial t} = -eE_x$.

To determine which fraction of the final k-box j stems from a given initial k-box, the vertices of the final box j are mapped onto the initial k-box using its linear energy interpolation. For transmission, the vertex energies are shifted by the potential difference between the adjacent Voronoi cells; for reflection, no energy shift is applied since the reflection flux originates from within the same spatial Voronoi cell. The geometric overlap between the initial k-box and the mapped final box is computed with the Sutherland–Hodgman algorithm [12], and the resulting overlap area times v_j' (of the initial k-box) gives the transmission and reflection coefficients. If an overlap polygon shares an edge with the initial k-box, the neighboring k-box across that edge is tested as an additional candidate, and the procedure repeats until all contributing initial k-boxes are identified.

If local extrema or saddle points yield multiple possible initial states that satisfy the interface conditions, conflicts between initial k-boxes may arise. To detect and resolve these, the reverse mapping is performed: all candidate initial k-boxes are mapped onto the final box j using the linear energy interpolation of the final k-box, yielding a partitioning of the final k-box with respect to the candidate initial k-boxes. Overlapping partition polygons indicate conflicts, which are resolved based on which k-box is reached first according to Newton's classical equation of motion: The "earlier" partitions are subtracted from the final box, and the transmission/reflection coefficient is recomputed using only the remaining part of the final k-box. If the remaining part of the final box is below a threshold of $10^{-13} \cdot \Omega_j$, the algorithm terminates to avoid mapping numerically degenerated polygons.

III. RESULTS

In Fig. 4 the drift velocity is shown for a homogeneous monolayer of MoS₂ as a function of the electric field E_0 , and a velocity overshoot occurs due to intervalley transfer (Fig. 5). (We successfully validated these results by comparison with an in-house MC simulator for 2D materials.) Owing to the stronger scattering and higher band energy of the Q-valley,

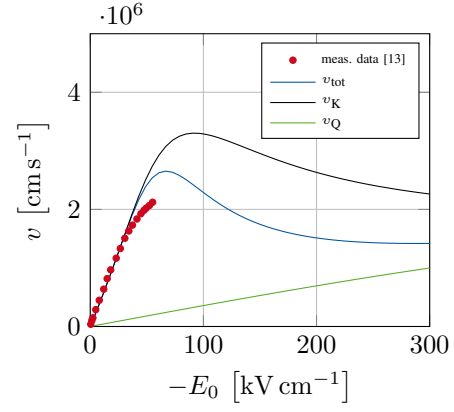


Fig. 4. Electron drift velocity v as function of the electric field E_0 for monolayer MoS₂ at $T = 300$ K, $N_{2D} = 1 \times 10^{12} \text{ cm}^{-2}$, and $N_c = 1.3 \times 10^{11} \text{ cm}^{-2}$ of the CC scattering was adapted to match μ_0 .

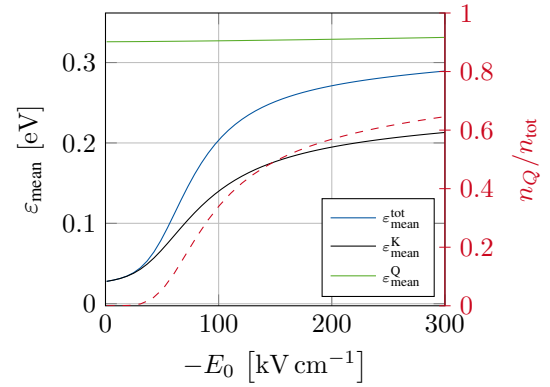


Fig. 5. Average energy w.r.t. the energy minimum of the K-valley and the occupation of the Q-valley (red curve) as function of E_0 for MoS₂.

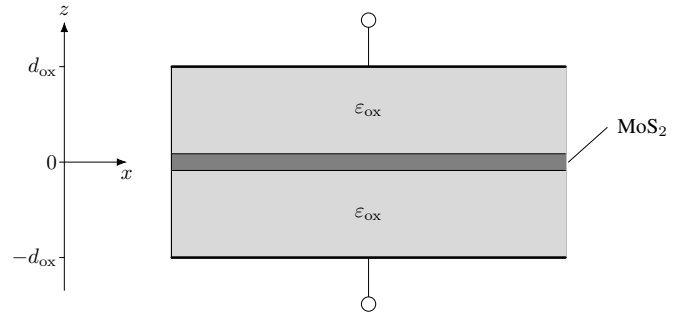


Fig. 6. Symmetric double-gate structure with a 2D material layer at $z = 0$.

its mean drift velocity v_Q is considerably lower, as shown in Fig. 4. However, the increasing K to Q intervalley transfer (red curve in Fig. 5) still increases the total mean energy because the Q-valley minimum energy lies 300 meV above that of the K-valley. To demonstrate the potential of the deterministic approach, we investigate the spatiotemporal small-signal case assuming plane-wave perturbations,

$$E(x, t) = E_0 + \text{Re}\{E \exp(st - iqx)\}, \quad (7)$$

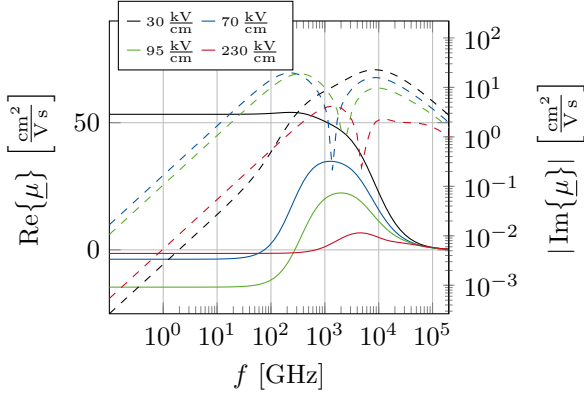


Fig. 7. Real part (solid curves) and imaginary part (dashed curves) of small-signal mobility for the DC electric fields $-E_0 = [30, 70, 95, 230] \frac{\text{kV}}{\text{cm}}$ for $q = 0$ in MoS_2 .

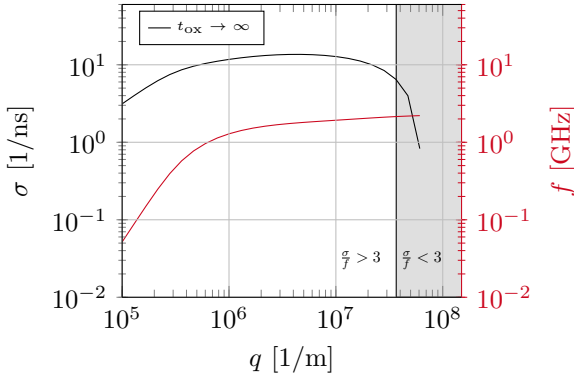


Fig. 8. Growth rate σ and frequency f of the soft plasma modes as a function of wave number q for monolayer MoS_2 with $-E_0 = 95 \text{ kV/cm}$. Kroemer's criterion is satisfied to the left of the gray area.

where E_0 is the DC electric field, $\underline{E}$ the phasor, $\underline{s} = \sigma + i2\pi f$, σ the growth constant of which positive values lead to plasma instabilities, f the frequency, and q the wave number. Fig. 7 shows the frequency dependence of the small-signal mobility $\underline{\mu}$ at $q = 0$, where the maximum of $\text{Re}\{\underline{\mu}\}$ is caused by the different energy and momentum relaxation times [14]. At low frequencies, $\text{Re}\{\underline{\mu}\}$ corresponds to the steady-state differential mobility and is negative for the three larger DC fields, enabling plasma oscillations. Since $\text{Re}\{\underline{\mu}\}$ is negative up to frequencies beyond 100 GHz, self-sustained oscillations might be possible at very high frequencies.

We therefore investigate for a symmetric double gate MOS structure consisting of MoS_2 and SiO_2 (see Fig. 6) soft plasma modes by their characteristic equation (for details see [14])

$$\underline{s} = -\frac{eN_{2D}q \tanh(qt_{\text{ox}})}{2\epsilon_{\text{ox}}} \underline{\mu}(\underline{s}, q), \quad (8)$$

where ϵ_{ox} is the permittivity of the oxide, t_{ox} its thickness, and N_{2D} the surface density of the electrons. Due to the 2D nature of the electron gas the growth constant σ first increases with q (Fig. 8) in contrast to the bulk case and then drops off at very high q . Kroemer's criterion for Gunn domain forming

($\sigma > 3f$) [15] is satisfied up to very large q leading to a peak oscillation frequency of 2.1 GHz at $q = 3.6 \times 10^7 \frac{1}{\text{m}}$ due to the low drift velocity (Fig. 4).

IV. CONCLUSION

We presented a deterministic full-band Boltzmann equation solver for 2D materials by extending a Godunov-type stabilization scheme to arbitrary band structures. For homogeneous MoS_2 , the solver predicts a distinct velocity overshoot and highlights the importance of full-band transport beyond the EMA. A small-signal analysis further indicates the possibility of soft plasma modes in MoS_2 , but further research is needed to confirm it. As in [8], the method can be extended straightforwardly to device simulations by coupling the Boltzmann equations across multiple spatial cells and applying appropriate contact boundary conditions.

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