

Lattice-Based Quantum Phonon Transport in FD-SOI Transistors

1st David Mai

Chair for Micro- und Nanoelectronics
TU Dortmund
Dortmund, Germany



2nd Dirk Schulz

Chair for Micro- und Nanoelectronics
TU Dortmund
Dortmund, Germany



Abstract—Thermal management in nanoscale ICs is increasingly challenged by the breakdown of semiclassical heat-transport models under strong spatial confinement. Specifically, conventional Boltzmann-based approaches are limited in capturing coherent phonon transport in advanced CMOS devices such as FD-SOI transistors. We present a computationally efficient lattice-based quantum framework based on a real-space density-matrix description. Exploiting sparse atomistic coupling, the method enables scalable, fully spatially resolved simulations, while a Wigner-Weyl transformation is used as a post-processing step to analyze phase-space coherence. Applied to 2D phonon transport in an FD-SOI transistor, the simulations reveal strong phonon confinement within the channel and pronounced coherent counter-propagating contributions. This reveals a direct relationship between device geometry and heat accumulation and highlights the relevance of spatially resolved quantum transport models for device-level thermal analysis. A purely ballistic framework is expanded to include diffusive phonon-phonon scattering. This creates a hybrid transport approach that balances quantum-coherent dynamics inside the nanostructure with realistic thermal relaxation at larger scales.

Index Terms—phonon transport, lattice dynamics, quantum transport, nanoscale devices, integrated circuits.

I. INTRODUCTION

Understanding phonon transport is crucial for the development of nanoscale semiconductor devices, such as thermal sensors based on low-dimensional structures, and for thermal and energy management in advanced integrated circuits [1], [2]. At these length scales, classical transport models become insufficient, as wave effects, coherence, and interface scattering strongly influence heat conduction, particularly in device architectures with layered material stacks.

Common approaches rely on Boltzmann-type transport equations [3], [4] or Wigner function formalisms [5], [6]. While Boltzmann methods provide an efficient semiclassical description, they neglect phase coherence between phonon modes and are therefore limited in nanoscale devices with strong spatial inhomogeneities. Wigner-based approaches, in contrast, can capture coherence effects, but their direct numerical implementation becomes computationally demanding and difficult to apply to realistic device geometries in integrated circuits. In this work, we introduce a real-space density-matrix formalism that enables an atomistic and discrete description of phonon transport in device-relevant structures. The method

naturally incorporates local variations such as material interfaces, confinement effects, and spatially varying coupling parameters typical for modern semiconductor technologies. A lattice-based quantum framework describing the ballistic phonon transport is expanded to incorporate diffusive transport regimes. While retaining the computationally efficient real-space description and full quantum coherence during ballistic propagation, we introduce a rigorous yet computable treatment of anharmonic phonon-phonon scattering. By systematically applying Wick's theorem, Born-Markov, and Random-Phase approximations, the multi-particle collision operator is mapped onto a scattering term in the eigenbasis. This establishes a versatile hybrid quantum-classical transport model capable of capturing both localized wave-like interference and macroscopic thermal relaxation in nanoscale devices. While the time evolution is efficiently computed through an eigenbasis, a Wigner-Weyl transformation is employed as a post-processing step to analyze the transport dynamics in phase space. The applicability of the approach is demonstrated by analyzing phonon transport in a Fully Depleted-Silicon-On-Insulator (FD-SOI) transistor.

II. MODEL

A. Ballistic Transport

To describe ballistic phonon transport in integrated circuits, lattice dynamics are formulated in real space within the framework of second quantization. This real-space representation is particularly advantageous for device-scale simulations, as it naturally leads to compact matrix operations and thereby enables efficient treatment of large, spatially inhomogeneous structures such as FD-SOI transistors.

The phonon system is described by a harmonic lattice Hamiltonian written in terms of creation and annihilation operators,

$$\hat{H}_{\text{ph}} = \sum_{l,m} d_{lm} \hat{a}_l^\dagger \hat{a}_m, \quad (1)$$

where the coupling matrix d_{lm} encodes nearest and next-nearest neighbor interactions in local space and thereby captures local material variations in a flexible manner. The time

evolution of the density matrix $\rho = \hat{a}_k^\dagger \hat{a}_l$ is governed by the von-Neumann equation

$$\partial_t \rho = -\frac{i}{\hbar} [\hat{H}_{\text{ph}} + \hat{H}_{\text{el-ph}}, \rho]. \quad (2)$$

In the present formulation, ballistic transport is obtained from the coherent real-space dynamics generated by $[\hat{H}_{\text{ph}}, \rho]$. The electron-phonon interaction $\hat{H}_{\text{el-ph}}$ acts as a local excitation mechanism and defines the initial driving of the system. This contribution is summarized by an excitation operator $\hat{S}$, leading to

$$\partial_t \rho = -\frac{i}{\hbar} [\hat{H}_{\text{ph}}, \rho] + \hat{S}. \quad (3)$$

Here, $\hat{S}$ denotes an effective static source term derived from a Redfield-type treatment [7] of the electron-phonon interaction and used in the present study to model phonon excitation.

To compute the time evolution efficiently, we transform the density matrix into the eigenbasis of the system. By diagonalizing the dynamic matrix, we obtain the eigenmodes with eigenvalues λ_q . The transformed density matrix $\tilde{\rho}_{kl}$ evolves according to:

$$\partial_t \tilde{\rho}_{kl} = i(\lambda_l - \lambda_k) \tilde{\rho}_{kl} + \tilde{S}_{kl}. \quad (4)$$

We employ a first-order exponential time differencing (ETD1) scheme [8]. Assuming a static source term, each time step is computed analytically:

$$\tilde{\rho}_{t+1} = \tilde{\rho}_t e^{i(\lambda_l - \lambda_k)\Delta t} + \tilde{S} \frac{e^{i(\lambda_l - \lambda_k)\Delta t} - 1}{i(\lambda_l - \lambda_k)}. \quad (5)$$

The numerical stability of the ballistic time evolution is strictly guaranteed by the properties of the real-space dynamical matrix. Due to its hermiticity, the diagonalization yields purely real and positive eigenvalues λ_q . Consequently, the exponent $i(\lambda_l - \lambda_k)\Delta t$ remains strictly imaginary, preventing unphysical exponential growth or damping during the coherent propagation step.

B. Diffusive Transport

To extend the model to diffusive transport, we include phonon-phonon scattering via an anharmonic Hamiltonian $\hat{H}_{\text{anh}}$:

$$\partial_t \rho = -\frac{i}{\hbar} [\hat{H}_{\text{ph}} + \hat{H}_{\text{anh}}, \rho] + \hat{S}. \quad (6)$$

This nonlinear scattering term introduces a hierarchy problem, where the time evolution of the 2-point density matrix operator couples to higher-order 3-point operators. To truncate this infinite hierarchy and to achieve a closed kinetic equation, approximations need to be applied. By using Wick's theorem at the hierarchy order involving 4-point operators, the 4-point expectation values are decomposed into products of 2-point operators, effectively mapping the system back onto the density matrix elements $\tilde{\rho}_{kl}$. The explicit time evolution of the 3-point operators inherently introduces a non-local temporal dependency, where the scattering rates depend on past scattering processes of the density matrix via a time-integral. By invoking the Markov approximation, it is assumed

that the correlation functions of the phonon bath decay on a significantly faster timescale than the macroscopic transport dynamics. This effectively eliminates the memory effects of past scattering events, resolving the temporal dependency of the 3-point operator and reducing the equation of motion to a time-local formulation only depending on the current state of the density matrix $\tilde{\rho}_{kl}(t)$. Mathematically, this temporal dephasing causes the unperturbed exponential propagation operators to transform into Dirac δ -functions, enforcing strict energy conservation for the three-phonon processes. By applying the Random-Phase Approximation (RPA), rapidly oscillating off-diagonal scattering matrix elements are eliminated, effectively neglecting phase coherences within the scattering environment. As a consequence, the scattering term couples predominantly to the diagonal elements $\tilde{\rho}_{ll}$, driving the system toward a Boltzmann-like collision phenomenology. Through these approximations, the time evolution of the density matrix can be expressed through

$$\begin{aligned} \partial_t \tilde{\rho}_{kl} = & i(\lambda_l - \lambda_k) \tilde{\rho}_{kl} + \tilde{S}_{kl} \\ & + \sum_{q_1, q_2} |V_{l, q_1, q_2}|^2 \{ \delta(\lambda_l - \lambda_{q_1} - \lambda_{q_2}) \\ & [\tilde{\rho}_{ll} \tilde{\rho}_{q_1 q_1} + \tilde{\rho}_{ll} \tilde{\rho}_{q_2 q_2} - \tilde{\rho}_{q_1 q_1} \tilde{\rho}_{q_2 q_2}] \\ & + 2\delta(\lambda_l + \lambda_{q_1} - \lambda_{q_2}) \\ & [\tilde{\rho}_{ll} \tilde{\rho}_{q_1 q_1} - \tilde{\rho}_{ll} \tilde{\rho}_{q_2 q_2} - \tilde{\rho}_{q_1 q_1} \tilde{\rho}_{q_2 q_2}] \}. \end{aligned} \quad (7)$$

Here, $\tilde{\rho}_{ll}$ denotes the diagonal elements of the phonon distribution function, $|V_{l, q_1, q_2}|^2$ describes the coupling matrix of the scattering events, and the conservation of energy is granted by the Dirac-delta-distribution. Due to the time locality of the scattering term, the time evolution can be resolved using a first-order operator splitting method [9]. The ballistic part is solved analytically via ETD1, while the scattering term is integrated using a fourth-order Runge-Kutta method.

This approach establishes a hybrid transport framework where quantum-coherent dynamics are preserved in the ballistic propagation, while the diffusive phonon-phonon scattering is treated in a controlled regime. The RPA suppresses inter-mode coherences so that the collision operators acts predominantly on the phonon populations (diagonal density elements), thereby recovering the structure of a Boltzmann collision integral. Unlike the conventional phonon Boltzmann equation, however, the scattering matrix elements V_{l, q_1, q_2} and the energy-conserving eigenvalues λ_l are evaluated in the global eigenmode basis of the entire, structurally inhomogeneous device. Consequently, the collision operator retains the intrinsic non-local character of the system eigenmodes while neglecting only inter-mode phase coherences. Therefore, while the scattering process itself is phase-insensitive, the phase-coherent structural wave properties are implicitly accounted for within the scattering kinematics.

The transition via the RPA is computationally indispensable. Retaining the full, non-local quantum-coherences within the multi-particle collision operator would introduce a prohibitive numerical overhead, rendering device-scale simulations of structures like FD-SOI transistors not computable. The pre-

sented hybrid approach thus avoids this computational bottleneck, balancing physical accuracy with numerical viability. Finally, the density matrix is back-transformed to real space and as a post-processing step, via a Wigner-Weyl transformation, transformed into spatial phase space to analyze the phase-space dynamics, while still preserving the computational advantages of the eigenbasis.

This approach establishes a hybrid transport framework where quantum-coherent dynamics are preserved in the ballistic propagation, while the diffusive phonon-phonon scattering is treated in a controlled, semiclassical regime. The RPA suppresses rapidly oscillating inter-mode coherences during the scattering event itself, so that the collision operator acts predominantly on the diagonal elements $\hat{\rho}_{ll}$. Consequently, it formally recovers the structure of a semiclassical Boltzmann collision integral.

Crucially, however, unlike the conventional phonon Boltzmann equation—which relies on bulk-like plane-wave states—our scattering matrix elements V_{l,q_1,q_2} and the energy-conserving eigenvalues λ_l are evaluated in the global eigenmode basis of the entire, structurally inhomogeneous device. Since these global eigenmodes are derived from the exact real-space harmonic lattice Hamiltonian, they inherently encapsulate the full spatial confinement, material interfaces, and geometric phase coherences of the FD-SOI transistor stacked architecture. Therefore, while the scattering process itself is phase-insensitive (population-driven), the phase-coherent structural wave properties are implicitly and rigorously accounted for within the scattering kinematics.

III. RESULTS

To evaluate the model, 2D ballistic phonon transport in a FD-SOI structure (Fig. 1) is investigated. A constant electron current is assumed, driven by a drain-source voltage of $U_{DS} = 0.1\text{ V}$ and a drain-source current of $I_{DS} = 10\text{ }\mu\text{A}$, which enters the electron-phonon coupling term in Eq. 3.

For the structural discretization, a uniform spatial grid of $n = 90$ points in both the x - and y -directions is employed, where the material-dependent lattice constants determine the discretization steps Δx and Δy . The time evolution is computed over 400 steps with a time step of $\Delta t = 50\text{ fs}$.

Figure 1 shows the resulting phonon density in real space. A pronounced hotspot is observed at the drain-side edge of the gate, where electrons reach maximum energy and most efficiently transfer energy to the lattice via electron-phonon coupling. Furthermore, phonon generation is strongly confined to the active channel region, with only weak leakage into the surrounding dielectric layers. To further analyze the transport mechanisms, a one-dimensional phase-space representation is extracted along the yellow line indicated in Fig. 1. Figure 2 reveals pronounced reflections at the material interfaces between channel and dielectric across a broad range of wave vectors. As a consequence, phonon transport remains largely confined within the channel region. At $y = 22\text{ nm}$, both positive and negative extrema in the phase-space distribution are observed. This can be attributed to coherent contributions

of counter-propagating phonon wave packets generated at the same spatial location, consistent with the excitation region shown in Fig. 1.

The identical device configuration and simulation parameters are subsequently evaluated under the inclusion of diffusive transport (Eq. 7). In Fig. 3 the phonon density is depicted across the FD-SOI transistor and Fig. 4 shows the scattering term for a single timestep. With the scattering term enabled, the macroscopic spatial profile of the phonon density remains closely aligned with the purely ballistic configuration due to the dominant geometric confinement of the FD-SOI stack, as depicted in Fig. 3. However, because the static source term continuously injects phonons spectrally uniform across all phonon branches into the channel, the local scattering rate increases significantly, triggering active microscopic relaxation pathways that are further resolved in Fig. 4. Due to the low group velocity of the high-energy acoustic and optical phonons, the three-phonon decay process ($l \rightarrow q_1 + q_2$) into lower-energy acoustic modes dominates within the channel, leading to a local accumulation of the total particle number. Following this decay, these low-energy acoustic phonons diffuse across the material interfaces into the surrounding SiO_2 dielectric. Since high-energy phonons are absent in the dielectric layers, the scattering physics there are dominated by the absorption process ($l + q_1 \rightarrow q_2$) mediated by the thermal background of the dielectric. This absorption mechanism reduces the local non-equilibrium particle number and effectively thermalizes the excess energy toward thermodynamic equilibrium.

IV. DISCUSSION AND CONCLUSION

The presented model provides a quantum-mechanical description of phonon transport in realistic device geometries and captures coherent phonon interference in phase space. Both the 2D real-space results and the phase-space analysis indicate pronounced phonon confinement within the FD-SOI channel due to reflections at the channel-dielectric interfaces. The reduced phonon out-diffusion leads to localized heat accumulation in the active region and thus contributes to self-heating in FD-SOI transistors. Through the inclusion of the anharmonic scattering term, especially in the channel region, three-phonon decay processes become visible. These processes scatter highly non-equilibrium phonons into lower-energy acoustic modes which subsequently diffuse into the surrounding dielectric, reducing the strict and artificial confinement seen in purely ballistic transport. By evaluating the scattering mechanics within the global system eigenbasis, this hybrid framework successfully balances atomistic quantum effects with macroscopic thermal relaxation, offering a computationally viable path for advanced device-level thermal analysis.

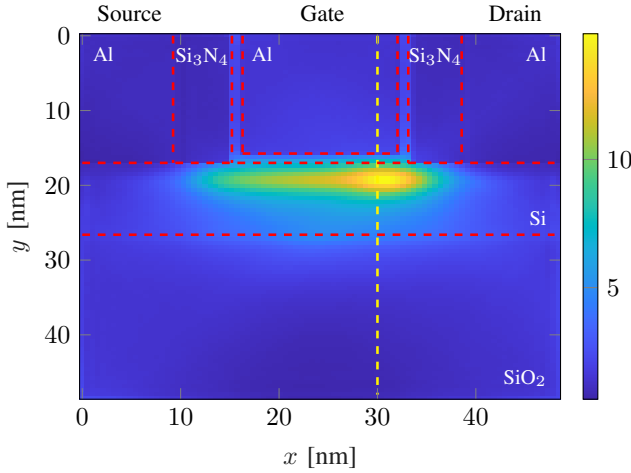


Fig. 1. The structure geometries of a FD-SOI-transistor are depicted. The phonon density at $t = 20$ ps is locally confined within the channel by dielectric layers, resulting in a high local phonon concentration. A maximum in phonon generation is observable at the drain-side edge of the gate.

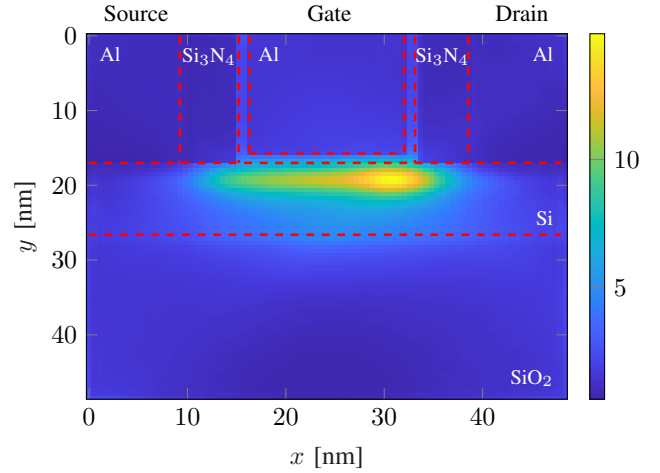


Fig. 3. Spatial phonon density distribution at $t = 20$ ps with inclusion of diffusive phonon-phonon scattering (Eq. 7). While the macroscopic spatial profile remains closely aligned with the purely ballistic configuration (Fig. 1) due to the dominant geometric confinement of the FD-SOI stack, the underlying microscopic relaxation mechanisms and mode conversions are governed by the local collision processes further resolved in Fig. 4.

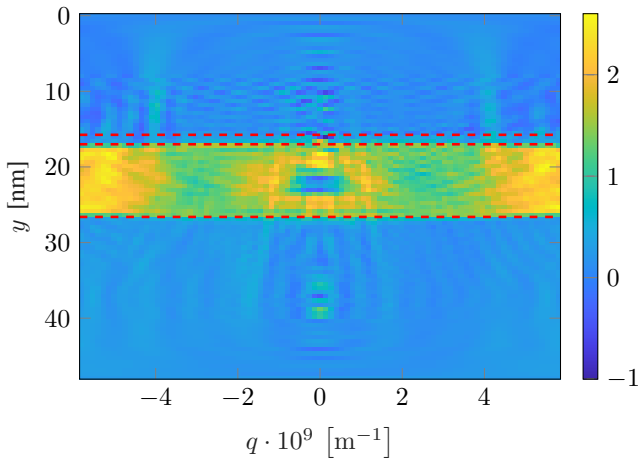


Fig. 2. Time evolution of the quasi-probability density matrix at $t = 20$ ps. Across all phonon modes q , strong confinement within the channel is evident, consistent with Fig. 1. Quantum mechanical effects are visible at the peak of phonon emission ($y = 22$ nm) as stationary quantum interference of phonon modes propagating in opposite directions.

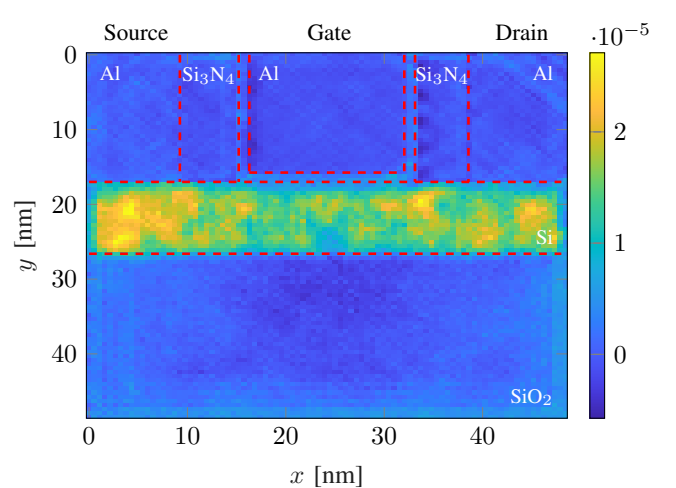


Fig. 4. Spatially resolved representation of the multi-particle scattering operator at a single time step. The plot illustrates the local transition from dominant three-phonon decay processes inside the highly non-equilibrium channel zone to localized phonon absorption near the SiO₂ interfaces, driving the energy relaxation toward thermodynamic equilibrium.

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