Importance of the Wigner equation for the analysis of the ballistic phonon transport

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Abstract— **Usually the computation of the ballistic phonon transport is approximated through Boltzmann type equations (BTE). Especially for hot electro-effects a more precise depiction of the phonon dispersion is needed to correctly apply processes like Umklapp scattering. This can be achieved through a Wigner transport equation (WTE) for phonons.**

Introduction

Mostly the Boltzmann equation is used to develop models for the phonon transport [1], even a Wigner equation has been proposed [2]. Those methods are using a linear approximation of the phonon dispersion resulting in an inaccurate representation of it. A precise depiction of the dispersion can be achieved through an inclusion of higher order phonon Hamiltonians into the Wigner equation. The phonon dispersion of acoustic phonons in homostructures and heterostructures is examined through BTE and WTE and those methods are compared. Of course optical phonons can be adressed with the proposed method.

Model

For demonstration purposes a Hamiltonian is introduced considering inversion symmetry, with which the von Neumann equation can be set up with coordinates r_1, r_2. Through the multiplication of the Hamiltonian with a locally varying function $s(r_1)$ and $s(r_2)$ respectivly, heterostructures can be described. We arrive at

$$\frac{\partial}{\partial t}\hat{\rho} = \sum_{n=0}^{N} c_n (s(r_1)\nabla_{r^1}^{2n} - s(r_2)\nabla_{r^2}^{2n})\hat{\rho} \qquad (1)$$

Utilizing a transformation onto center of mass coordinates r, r', the Wigner-Weyl transformation results into the formulation of a Wigner function $f(r, k)$ in the phase space. The Boltzman equation can be established through the consideration of only the first order derivative in eq. (1). A central differencing scheme is used in r-direction. The boundary condition in the real space are set through Perfectly Matched Layers (PML) [3] and a transient calculation is achieved using matrix exponantials, which can be approximated by applying Model Order Reduction methods like Krylow-subspace methods.

Results

A simple Si material for homostructures and a Si/SiGe-junction are being used to compare the mentioned BTE and WTE. The latter material system can be found in Hetero-Bipolar-Transistors (HBT) for instance. The Wigner function of the phonons is shown in Fig. 1 using the Boltzmann equation and in Fig. 2 using phonon Hamiltonians up to the third order as for example. Especially near the edges of the first Brillouin zone differences between these approaches can be seen. While Fig. 2 displays a precise depiction of the phonon dispersion, the Boltzmann equation only shows a linear dependence on k. A similar behaviour can be seen from Fig. 3 and Fig. 4 for heterojunctions.

Conclusion

The use of a Wigner transport equation is needed to precisely reproduce the phonon dispersion especially near the edges of the first Brillouin zone as needed in investigations linked with processes when the nonballistic phonon transport is considered.

References

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[2] Simoncelli, M. and Marzari, N. and Mauri, F., *Wigner Formulation of Thermal Transport in Solids*, PhysRev X 12, 041011 (2022)
[3] Steven G. Johnson, *Notes on Perfectly Matched Layers (PMLs)*, arXiv, 2108.05348 (2021).

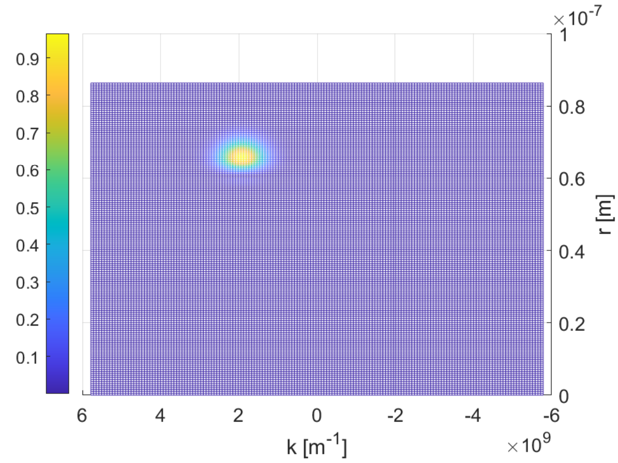

Fig. 1. A Gaussian distribution is set for all k in a Si material. The propagation of $f(r, k)$ using the BTE is shown. The yellow surface indicates the maximum of the distribution while the blue surface indicates a minimum. A linear dependence on k is visible.

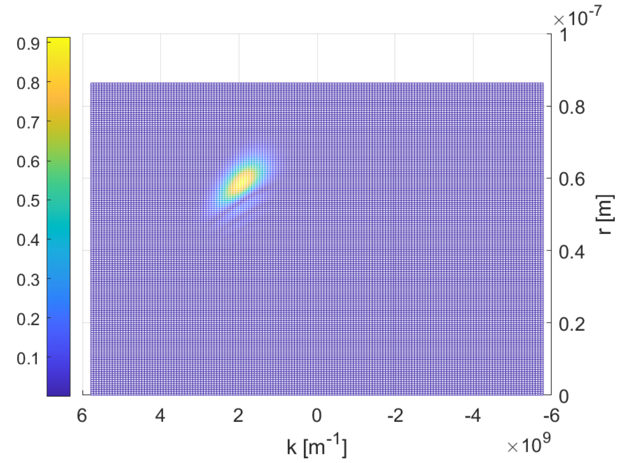

Fig. 2. A Gaussian distribution is set for all k in a Si material. The propagation of $f(r, k)$ using the WTE including Hamiltonians up to the third order is shown. The yellow surface indicates the maximum of the distribution while the blue surface indicates a minimum. The phonon dispersion towards the edges of the k-grid is visible.

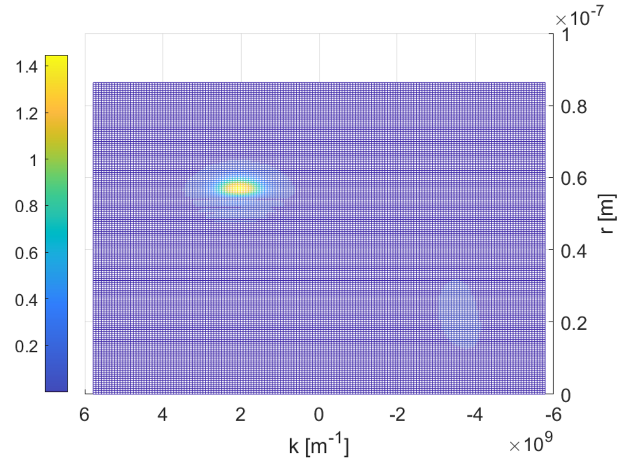

Fig. 3. A Gaussian distribution is set for all k in a Si/Si$_{0.9}$Ge$_{0.1}$ junction. The junction is set in the middle of the r-grid at 43nm. The propagation of $f(r, k)$ using the BTE is shown. The yellow surface indicates the maximum of the distribution while the dark blue surface indicates a minimum. Similar to the distribution in Fig. 1 a linear dependence on k is visible. However, through the junction an increasing maximum is shown and a part of the distribution is reflected, seen at the edges of the k-grid in light blue. The propagation velocity also decreases in the SiGe material.

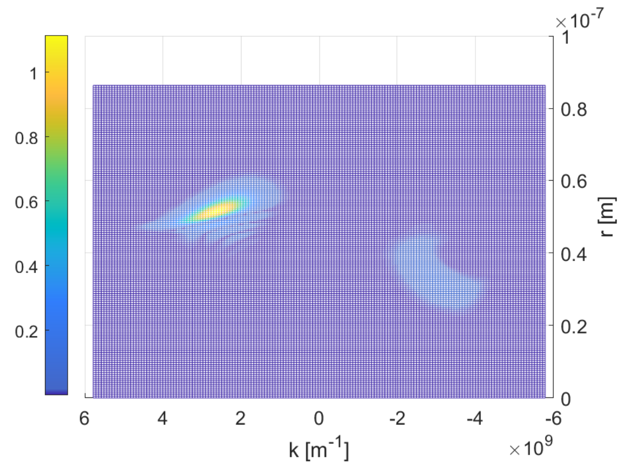

Fig. 4. A Gaussian distribution is set for all k in a Si/Si$_{0.9}$Ge$_{0.1}$ junction. The junction is set in the middle of the r-grid at 43nm. The propagation of the waves using the WTE is shown. The orange/yellow surface indicates the maximum of the distribution while the dark blue surface indicates a minimum. Similar to the distribution in Fig. 2 and in contrast to Fig. 3, the phonon dispersion is visible. However, through the junction a small increase of the maximum is shown and a part of the distribution is reflected, seen at the edges of the k-grid in light blue. The propagation velocity also decreases in the SiGe material as in Fig. 3 for the BTE.