MATHEMATICAL CHALLENGES IN CHARGE TRANSPORT WITHIN LOW DIMENSIONAL MATERIALS

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ABSTRACT

In recent years, two-dimensional (2D) materials have attracted considerable attention owing to their wide-ranging potential applications [**?**]. Among these, graphene has emerged as one of the most extensively investigated candidates, being regarded as a promising material for integration into nanoelectronic and optoelectronic devices; in fact, this represent the ultimate miniaturization since the active area is only one atom tick. The description of charge transport in graphene can be formulated at different levels of physical complexity [**?**]. At the quantum scale, the Wigner equation provides an accurate theoretical framework; however, in many situations its semiclassical counterpart, the Boltzmann equation, is a very good model. The substantial numerical challenges associated with solving either the Wigner or the semiclassical Boltzmann equation have motivated the development of alternative macroscopic approaches, including hydrodynamic, energy-transport, and drift–diffusion models. These models are particularly relevant in the context of designing next-generation electronic devices in which graphene may replace conventional semiconductors such as silicon and gallium arsenide. Thermal phenomena in low-dimensional structures also play a critical role, necessitating the incorporation of phonon transport through the Peierls–Boltzmann equation for each phonon branch. Furthermore, uncertainties in key material parameters—such as the effective band gap and the magnitude of the applied electric field—introduce significant variability in the predicted charge transport properties of graphene nanoribbons [**?**; **?**]. These challenges give rise to novel mathematical problems directly linked to the distinctive physical features of graphene. The principal aspects will be examined, and recent advances [**?**; **?**; **?**; **?**; **?**; **?**; **?**] will be presented in the broader perspective of future developments, with particular emphasis on the design and optimization of graphene-based field-effect transistors and on the rigorous treatment of uncertainty quantification in graphene nanoribbons [**?**].

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