Simulation of Klein-tunneling in Graphene

using Summation-by-Parts-Simultaneous Approximation Term (SBP-SAT)

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Summary

- Simulation of massless Dirac fermions in graphene.
- Calculation of the transmission probability of fermions across a potential barrier as a function of the angle of incidence.

Klein-tunneling is a relativistic quantum mechanical phenomenon which consists in a particle traveling through a potential barrier with certainty, regardless of the height and the width of the barrier.

Electrons in graphene can be described as massless Dirac fermions. Their behavior is modeled by the equation

$$i\hbar\psi_t = -i\hbar\sigma\nabla\psi + V_0\psi. \quad (\blacklozenge)$$

The discretization of (♦) is made with a sixth order SBP-SAT method in the spatial domain while for time integration a fourth order Runge Kutta scheme is used. The method is proven to be strictly stable for ingoing characteristic boundary conditions.

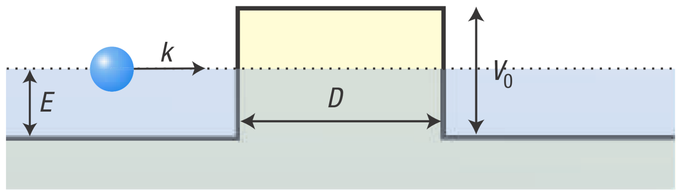

Figure 1. A particle with energy E and momentum k traveling towards a potential barrier of width D, energy V_0.

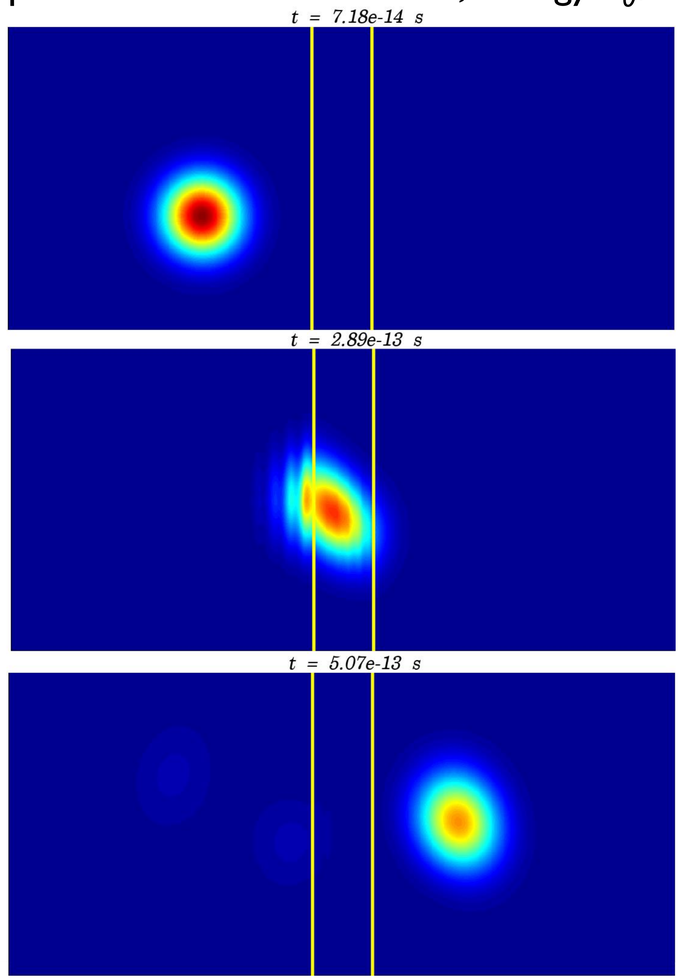

Figure 2. Probability function of a massless Dirac fermion hitting a potential barrier at an angle of 15°, illustrated by a Gaussian wave-packet, at different times.

The aim of this project is to compare the theoretical plane wave time-independent solutions to (♦) and its dynamical solutions with an actual particle traveling through a potential barrier.

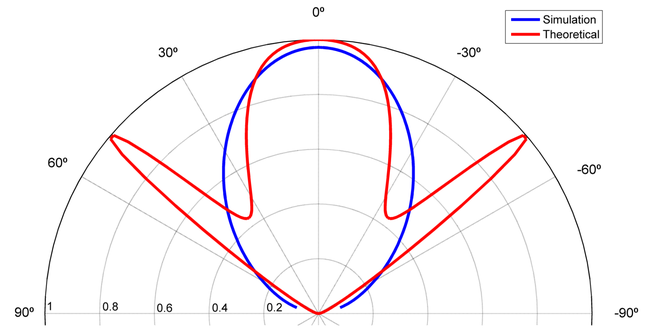

Figure 3. Transmission probability as a function of the angle of incidence.

Conclusions The numerical time-dependent simulations do not agree with the theoretical stationary results. This discrepancy in the transmission probability may be justified by the fact that, instead of plane waves, we model our particles more realistically as moving wave-packets.

References

M. I. Katsnelson, et al. Chiral tunnelling and the Klein paradox in graphene. *Nature Physics*, 2(9):620-625, August 2006.