QUANTUM LATTICE BOLTZMANN SIMULATION OF CHARGE CARRIERS IN GRAPHENE

D. Lapitski[a*] and **P. J. Dellar**[a*]

[a]OCIAM, Mathematical Institute, University of Oxford, Oxford, United Kingdom
*Corresponding authors: *lapitski@maths.ox.ac.uk*, *dellar@maths.ox.ac.uk*

We use the quantum lattice Boltzmann (QLB) algorithm to simulate the behaviour of charge carriers in graphene, including simulations of free wavepackets and the Klein paradox. Proposed by Succi & Benzi [1,2], the QLB algorithm offers a discretisation of the Dirac equation that is unitary, unconditionally stable, and free of the fermion doubling problem. It shares many properties with the hydrodynamic lattice Boltzmann method (LBM) such as ease of parallelisation, and ease of implementation on graphics processing units (GPUs). In recent work we have demonstrated the ability of the QLB algorithm to capture solutions of the full Dirac equation, rather than just its non-relativistic limit the Schrödinger equation, in one, two, and three spatial dimensions [3,4]. We have also extended the algorithm to global second order accuracy, and to vector as well as scalar potentials. As well as their usual role to describe coupling to magnetic fields, vector potentials model the effects of strain in the graphene lattice [6,7].

We first present simulations of tunnelling by massless charge carriers relevant to monolayer graphene in two dimensions. This system is equivalent to one-dimensional tunnelling of particles with an effective mass given by the conserved component of the momentum transverse to the potential barrier [5]. The simulation results, along with theoretical transmission coefficient values, are shown in Figure 1 below. We obtain an exact solution for wavepackets using a superposition of analytical plane wave solutions, and show that our QLB solutions converge with second order accuracy to this exact solution. We also simulate evolution of free wave packets in two dimensions under different initializations of the relative phase of the two wave function components [8], as shown in Figure 2, and wave packets undergoing Klein tunnelling to observe the dependence of the transmission coefficient on the angle of incidence. In future work, we will use the QLB to simulation charge carriers with non-zero effective mass in graphene ribbons, and other modified forms graphene. In particular, band gaps opened using strain engineering act as an apparent uniform magnetic field [6,7] while ripples in the graphene lattice convert an applied uniform in-plane magnetic field into a spatially varying out-of-plane field [9]. Both these effects may now be modeled with the QLB algorithm [10].

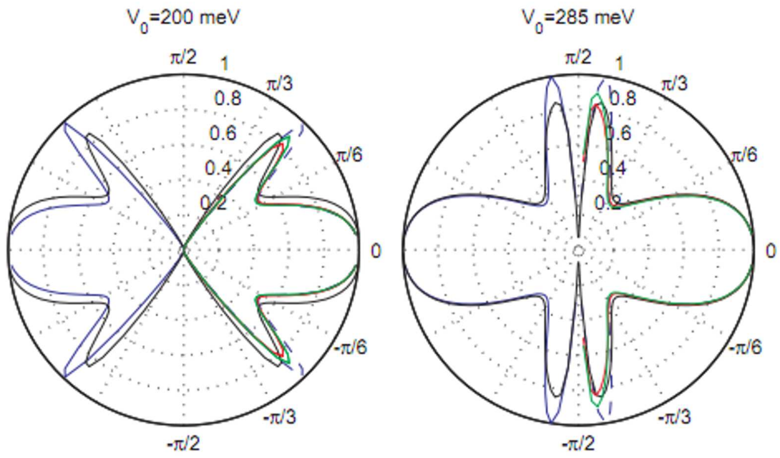

Figure 1: Simulated wave packet transmission as a function of angle of incidence in a one-dimensional representation of Klein tunnelling. Compare with Figure 2 in [5]

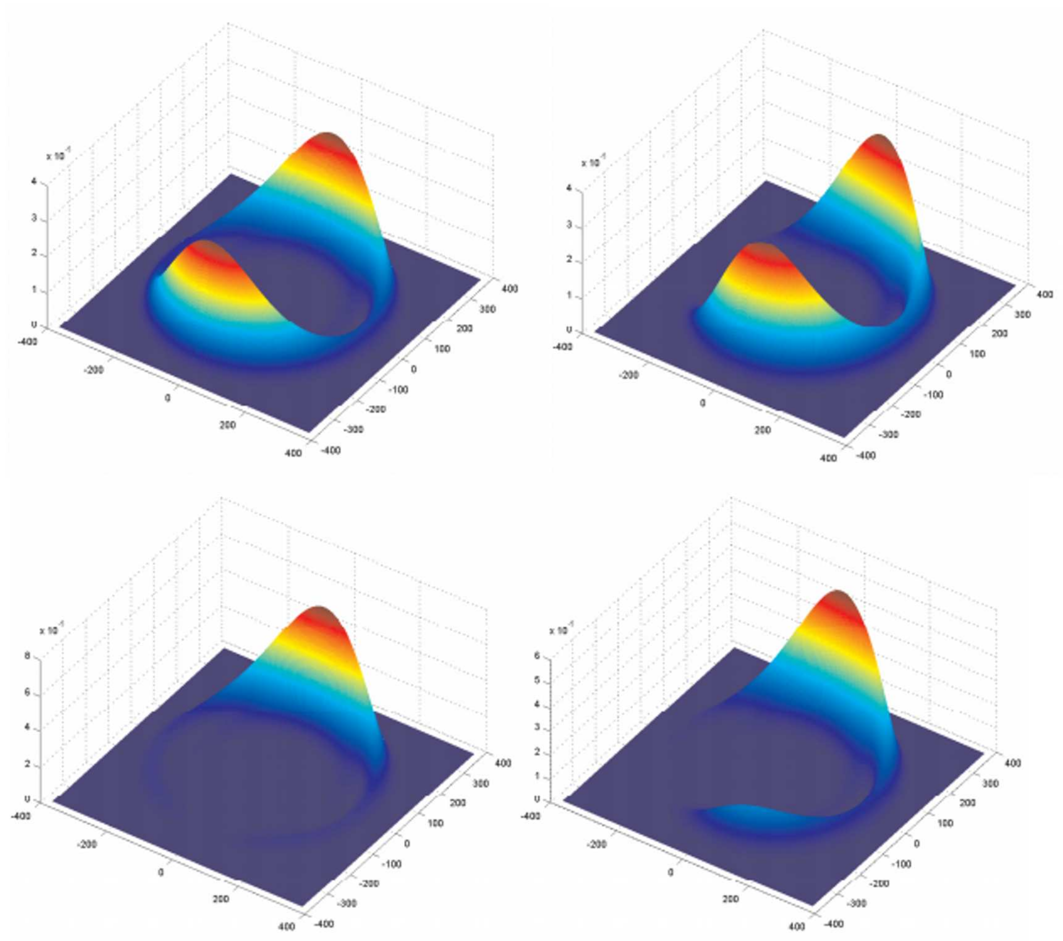

Figure 2: Evolution of free wave packets from different sets of initial conditions (as in [8]).

References

[1] S. Succi and R. Benzi, Physica D, 69 (1993) 327-332.
[2] S. Palpacelli and S. Succi, Commun. Comput. Phys, 4 (2008) 980-1007.
[3] D. Lapitski and P. J. Dellar, Convergence of a three-dimensional quantum lattice Boltzmann scheme towards solutions of the Dirac equation, Phil. Trans. R. Soc. Lond. A (to appear).
[4] P. J. Dellar, D. Lapitski, S. Palpacelli and S. Succi, A note on the isotropy of three-dimensional quantum lattice Boltzmann schemes, Phys. Rev E (to appear).
[5] M.I. Katsnelson, K.S. Novoselov, and A.K. Geim, Nature Phys., 2 (2006) 620-625.
[6] F. Guinea, M. I. Katsnelson, and A. K. Geim, Nature Phys., 6 (2010) 30-33.
[7] A.H. Castro Neto, F. Guinea, N.M.R. Peres, K.S. Novoselov, and A.K. Geim, Rev. Mod. Phys., 81 (2009) 109-162.
[8] G.M. Maksimova, V.Ya. Demikhovskii, and E.V. Frolova, Phys. Rev. B, 78 (2008) 235321.
[9] M.B. Lundeberg and J.A. Folk, Phys. Rev. Lett., 105 (2010) 146804.
[10] This research is supported by an EPSRC Advanced Research Fellowship, grant number EP/E054625/1, held by PJD. DL is supported by a project studentship attached to the same grant.