

Vortex flows in semiconductor device quantum channels: time-dependent simulation

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Recently it has been proposed that the formation of blocking quantum vortices embedded in the open current flows between source and drain plays a significant role in determining the current-voltage characteristics of nano-scaled semiconductor devices [1, 2]. These studies were based on time-independent quantum transport models. The vortices are associated with angular momentum generation at non-uniformities in the channel, quantum interference with atomistic impurity distributions and surface roughness scattering. We find that generally the vortex cores lie on curved lines in three dimensions which thread the through the channel either as closed loops or open lines. In the present paper we report investigation of the physics of formation of vortices in time-dependent flows. This problem is crucial to quasi-ballistic channels where transient response is a more appropriate model for the current and density fields than asymptotic stationary state analysis. Preliminary results of application to ultra-small MOSFET devices are also reported.

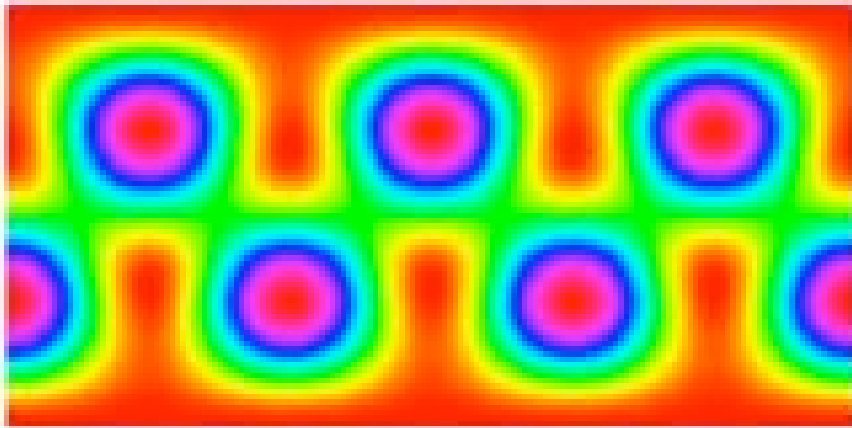
Whilst non-equilibrium Green function methods have been very successful in modeling very small devices they have involved the energy dependent (i.e stationary) Green functions. We first note that moving vortices may arise readily even in uniform systems when one considers non-stationary states. An example of an exactly soluble model is shown in Figure (1) where we see the generation of a moving vortex street in a uniform quantum channel arising from an initial excitation of the ground and first excited transverse states. The angular momentum generation is associated with the “sloshing” motion of a wave-packet between the channel walls. The decoherence of this process is not straightforward since quantized angular momentum states are difficult to destroy. We have studied this problem using a phenomenological model for the phase-breaking. This example is also investigated using the Green function formalism, where we formally build the time-dependent Green function from a Fourier transform over the energy-dependent Green functions. In this case we may transform to a coordinate frame that is co-moving with the vortex street to reduce the problem to an equivalent time-independent problem. As a second example we have used a similar construction together with our previous analytical steady-state (but non-asymptotic) Green function model for atomistic scattering [3] to construct a picture of the time-dependent scattering of a wave-packet on a discrete cluster of impurities. The results compare favourably with numerical Green function simulation provided the scattering is treated without self-averaging assumptions, i.e treated non-perturbatively. This poses a significant burden on the numerical computation: for realistic channels the model is forced to be 3D rather than 2D. A central goal of the present work is to understand how the stationary vortex flows at different energies superpose to produce the net flow in both the steady-state and time-dependent regimes. Preliminary results are presented for the onset of vortices when the fluctuation potential landscape of a rough interface is marginally changed for example by charge trapping.

[1] J. R. Barker, *Physica E* 19, 62 (2003); *J.Comp. Electronics*, 2, 153 (2003); *Semiconductor Science and Technology*, 19, S56 (2004); *Superlattices and Microstructures*, in the press (2004).

[2] M. V. Fischetti, S. E. Laux, A. Kumar, *IEEE Int. Electron Devices Meeting - Technical Digest.* , IEEE. , p.467-70 in 2003

A full journal publication of this work will be published in the *Journal of Computational Electronics*.

(a)



(b)

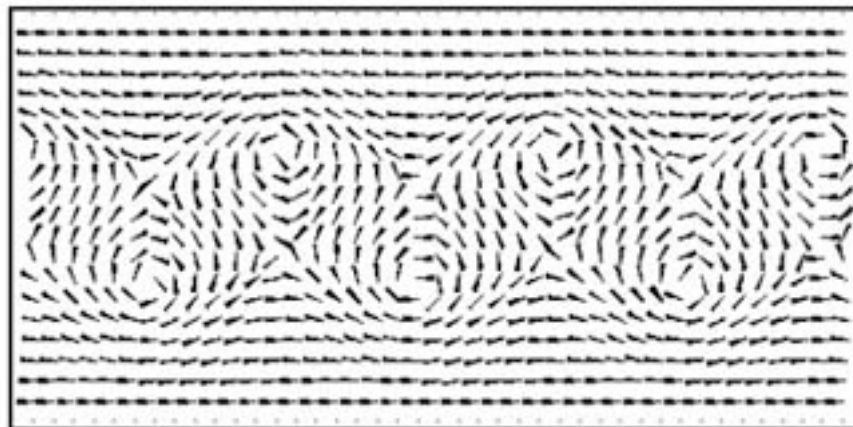
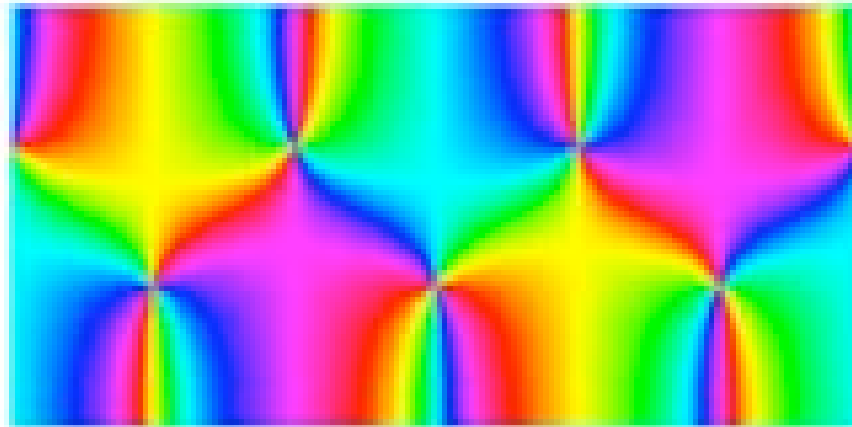


Figure 1 : 2D vortex street in moving frame of reference in a quantum channel: (a) density $n(\mathbf{r})$; (b) phase $S(\mathbf{r})$; (c) velocity field $\mathbf{v}(\mathbf{r})$ over a cross-section through the central vortex.