Time-dependent electromagnetics of molecular junctions

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In this talk, I will give an overview of recent developments in fast calculations of transient effects in quantum electronics using the time-dependent Landauer-Büttiker (TDLB) formalism [1]. First I discuss the generic model of a molecular junction described within the nonequilibrium Green's function (NEGF) framework. The switch-on of an arbitrary bias voltage is described in the case of both (i) the partitioned quench and (ii) the partition-free approach, which includes the effects of the pre-quench thermalization in the electronic response.

Within the TDLB, it is possible to derive analytic expressions for the first and second moments of the current for an arbitrary molecule described by a tight-binding Hamiltonian. I discuss how these are computed, and I propose a tight relationship between the current cross-correlations to the time taken for electrons to traverse the molecule [2,3].

Usually the sole concern of quantum transport calculations lies with currents, current noise and particle densities. However, it is possible to reverse this logic and instead use the molecular electronic currents as source terms for the local time-dependent electromagnetic fields. Recent work has shown how to do this, using a combination of the TDLB and Jefimenko's generalization of the Biot-Savart law [4]. As an application of this method, I present calculations done on benzene ring molecules in the ortho, para and meta configurations. The quantum interference between electron pathways can lead to a sign reversal of local currents and a strong switching effect in the local magnetic fields. I also present calculations of the emitted power in the field, showing that quantum effects should be detectable in the local radiation profile of the molecule.

[1] Ridley, M., MacKinnon, A., & Kantorovich, L. (2015). Current through a multilead nanojunction in response to an arbitrary time-dependent bias, Physical Review B, 91(12), 125433

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[3] Ridley, M., Sentef, M. A., & Tuovinen, R. (2019). Electron traversal times in disordered graphene nanoribbons, Entropy, 21(8), 737

[4] Ridley, M., Kantorovich, L., van Leeuwen, R., & Tuovinen, R. (2021). Quantum interference and the time-dependent radiation of nanojunctions, Physical Review B, 103(11), 115439