# INELASTIC EFFECTS IN ELECTRONIC CURRENTS :
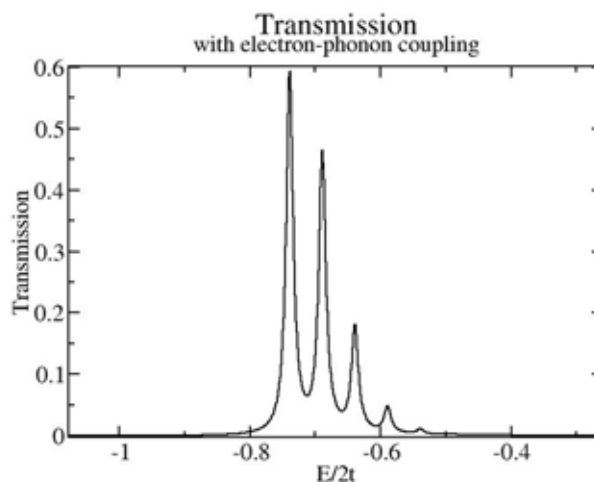# A TIME-DEPENDENT APPROACH

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The study of inelastic efects in electronic curents is receiving much attention due to both technological impact (molecular electronics are an emerging field in nanosciences) and the fundamental understanding of physics. From a theoretical point of view, the description of the mutual interaction between atomic vibrations and electrons leads to the development of sophisticated methods that use heavy formalism essentially based on non-equilibrium Green's functions (1). We have developed a method to the treat electron-phonon coupling to all orders in a time-dependent approach. We show that this simple method is a convenient tool to understand electronic transport in the presence of vibrations. Indeed, wave-packet propagation appears to be an intuitive and efficient way of describing phenomena such as inelastic electron tuneling spectroscopy. We will present a one-dimensional tight-binding model, and show how transmission can be calculated with wave-packets. Finally, some results will be discussed in the context of inelastic electron spectroscopy.

We consider a tight-binding one-dimensional chain, described by a tri-diagonal hamiltonian. Each site has equal on-site energy except one or several sites, wich we term « impurity sites ». A wave-packet is generated on the left side of the chain, with an initial kinetic energy. It propagates freely until the impurity sites are reached. There, it is reflected and transmitted, due to elastic scattering. If we switch on the electron-phonon coupling in the impurity sites, inelastic effects can be detected.

Time evolution of a wave packet
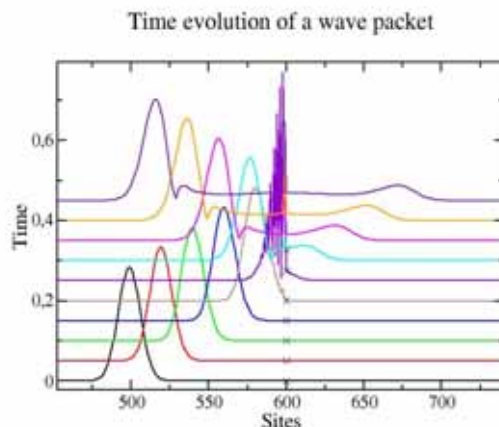
Transmission can be calculated using virtual detectors. The weight of the wave-function is calculated after the impurity sites as a function of time. Using a Fourier transform, we can compute the probability of an electron to be transmitted as a function of its initial energy. The width of the wave-packet is chosen so as to describe the appropriate spectral region where inelastic effects occur. In the presence of vibrations, the shape of the transmission curve is not loretzian anymore. The results show several peaks, spaced by the energy of the phonon, which are termed « phonon sidebands ». They correspond to the opening of additional channels of conductance.

Transmission
with electron-phonon coupling

Transmission (y-axis: 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6)
E/2t (x-axis: -1, -0.8, -0.6, -0.4)

The propagation is performed with the Lanczos algorithm (2), wich allows big time steps, rapid convergence, and flexibility in the implementation of the hamiltonian matrix. This last point is extremely important because, as our method permits us to calculate transmissions with an arbitrary number of phonons, we will need to increase the number of phonons until convergence is reached.

We think that this time dependent approach can provide intuitive explanations of the physics involved in inelastic scattering experiments. Moreover, the efficiency of the calculation shows that for single-electron problems, the physics can be understood with simple approaches like ours, wich are nevertheless capable to show the underlying complexity of the systems where vibrations play an important role in conductance properties (3).

(1) T. Frederiksen, M. Brandbyge, N. Lorente and A.-P. Jauho , Phys. Rev. Letters 93, 256601 (2004).
(2) S; Mahapatra and N. Sathyamurthy, J. Chem. Soc., Faraday Trans., 93, 773 (1997).
(3) M. Berthe, A. Urbieta, L.M.A. Perdigão, B. Grandidier, D. Deresmes, C. Delerue, D. Stiévenard, R. Rurrali, N. Lorente, L. Magaud, P. Ordejon, Phys. Rev. Lett. 97, 206801 (2006)