

Abstract Submitted  
for the MAR07 Meeting of  
The American Physical Society

**GW electronic Correlations in Quantum Transport : Renormalization and finite lifetime effects on real systems** PIERRE DARANCET, LEPES-CNRS and Université Joseph Fourier, Grenoble, ANDREA FERRETTI, Dipartimento di Fisica, Università di Modena e Reggio Emilia, and INFM-CNR-S3, National Center on nanoStructures and bioSystems at Surfaces, 41100, DIDIER MAYOU, VALERIO OLEVANO, LEPES-CNRS — We present an *ab initio* approach to electronic transport in nanoscale systems which includes electronic correlations through the GW approximation. With respect to Landauer approaches based on density-functional theory (DFT), we introduce a physical quasiparticle electronic-structure into a non-equilibrium Green's function theory framework. We use an equilibrium non-selfconsistent  $G^0W^0$  self-energy considering both full non-hermiticity and dynamical effects. The method is applied to a real system, a gold mono-atomic chain. With respect to DFT results, the conductance profile is modified and reduced by to the introduction of diffusion and loss-of-coherence effects. The linear response conductance characteristic appear to be in agreement with experimental results.

Pierre Darancet  
LEPES-CNRS and Université Joseph Fourier, Grenoble

Date submitted: 05 Dec 2006

Electronic form version 1.4