Applying Time-dependent DMRG to Calculate the Conductance of Nanostructures

KHALED AL-HASSANIEH, Oak Ridge National Laboratory, Oak Ridge TN, and University of Tennessee, Knoxville TN 37831, A. E. FEIGUIN, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106, J. A. RIERA, Universidad Nacional de Rosario, Avenida Pellegrini 250, 2000-Rosario, Argentina, C. A. BÜSSER, Ohio University, Athens, OH 45701, E. DAGOTTO, Oak Ridge National Laboratory, Oak Ridge TN, and University of Tennessee, Knoxville TN 37831 — DMRG provides a powerful tool to study quantum 1D systems. We present a detailed procedure for applying the recently developed time-dependent DMRG to calculate the conductance of nanostructures, such as quantum dots (QD’s). The leads are modelled using tight-binding Hamiltonians. The ground state at time zero is calculated at zero bias. Then a small bias is applied between the two leads, the wave-function is evolved in time and the current is measured as a function of time. Typically, the current saturates at a steady state after a short period of time. The conductance is obtained from the steady-state current. To test this approach we study several cases of interacting and non-interacting systems. Our results show excellent agreement with the exact results in the non-interacting case. We also reproduce quantitatively the well-established results in the case of one interacting QD and two coupled interacting QD’s. [1] K. A. Al-Hassanieh et al, in preparation. [2] Steven R. White and Adrian E. Feiguin, Phys. Rev. Lett. 93, 076041 (2004).

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