Photoexcitations in a 1D manganite model: From quasiclassical light absorption to quasiparticle relaxations¹ T. KÖHLER, O. SCHUMANN, F. BIEBL, S. KRAMER, S. KEHREIN, S. MANMANA, Inst. f. Theo. Phys., U. Göttingen, Germany, S. RAJPUROHIT, M. SOTOUEH, P. BLÖCHL, Inst. f. Theo. Phys., TU Clausthal, Germany — We investigate 1D correlated systems following a photoexcitation by combining ab-initio methods, time-dependent matrix product state (MPS) approaches, analytical insights from linearized quantum Boltzmann equations (LBE), and molecular dynamics (MD) simulations to describe the dynamics on different time scales ranging from femto- up to nanoseconds. This is done for manganite systems in the material class Pr$_{1-x}$Ca$_x$MnO$_3$. We derive 1D ab-initio model Hamiltonians for which we compute the ground states at different values of the doping using MD simulations. At half doping, we obtain a magnetic microstructure of alternating dimers from which we derive a 1D Hubbard-type model. The dynamics is analyzed concerning the formation and lifetime of such quasiparticles via a LBE. We find that the magnetic microstructure strongly enhances the lifetime of the excitations. In this way, our work constitutes a first step to building a unifying theoretical framework for the description of photoexcitations in strongly correlated materials over a wide range of time scales, capable of making predictions for ongoing experiments investigating pump-probe situations and unconventional photovoltaics.

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