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Kadanoff-Baym-Keldysh-Ehrenfest dynamics of correlated materials responding to ultrafast laser pulses LAZAR KISH, ROLAND ALLEN, Texas A&M University — In our many earlier simulations of the response of materials and molecules to laser pulses, one-electron states were determined by the time-dependent Schrödinger equation with an instantaneous one-electron Hamiltonian. These states were then used with Ehrenfest's theorem in a semiclassical treatment of the coupled dynamics of electrons and nuclear coordinates. For strongly-correlated materials, however, true nonequilibrium self-energies are required. Here we describe a practical numerical procedure for employing the Kadanoff-Baym/Keldysh equations together with Ehrenfest's theorem. In preliminary work we treat the simplest possible model of a system in which there is the potential for both a Peierls structural transition (involving doubling of the unit cell) and a Mott-Hubbard electronic transition (involving electron correlations). These calculations are relevant to understanding the dynamics of insulator-metal phase transitions in VO_2, which has been studied in ultrafast pump-probe measurements [1-3] and nanoscale imaging [4].

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