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Kadanoff-Baym-Keldysh-Ehrenfest dynamics of correlated materials responding to ultrafast laser pulses 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[1] together with Ehrenfest's theorem, and with conserving self-energies appropriate to correlated materials.

[1]See e.g. A. Stan, N. E. Dahlen, and R. van Leeuwen, J. Chem. Phys. 130, 224101 (2009) and T. Kita, Prog. Theor. Phys. 123, 581 (2010).

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