Theory of time-resolved photoemission spectroscopy

James Freericks[1], Wen Shen[1], Brian Moritz[2], Thomas Devereaux[2, 3], and Hulikal Krishnamurthy[4]

[1] *Department of Physics, Georgetown University, 37th and O Sts. NW, Washington, DC, 20057, USA*

[2] *Stanford Institute for Materials and Enrgy Science, SLAC National Laboratory, Menlo Park, California, 94025, USA*

[3] *Geballe Laboratory for Advanced Materials, Stanford University, Stanford, California, 94305, USA*

[4] *Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore, 560012, India*

In this talk, I will present a brief summary of the nonequilibrium many-body formalism for time-resolved (pump/probe) photoemission spectroscopy [1,2]. This formalism uses a straightforward evolution of the system along the Kadanoff-Baym-Keldysh contour with contour-ordered Green's functions which can be calculated exactly using dynamical mean-field theory. The photoemission spectra results from a two-time Fourier transform of the lesser Green's function, appropriately weighted by the probe pulse profile. I will next give examples of how one can use this technique to either see the evolution of the density of states from equilibrium to nonequilibrium (when driven by a constant pump) [3] or to see how the system evolves when driven by a pump and allowed to relax via many-body interactions (but no reservoir) [4]. In this latter case, one can see how the hot electron model is a good, but not perfect approximation. If time allows, I will also present results for what happens in a driven charge-density-wave phase at zero temperature (which has no relaxation processes), where the response after the pump cannot be easily described by a simple hot electron model. This latter effect arises from the fact that the order parameter can oscillate in time, yielding an oscillatory current in the "steady state". For photoemission, we see a decoupling of the phenomena of gap closure versus vanishing of the order parameter, hence the "melting" of a charge-density-wave insulator is more complicated in nonequilibrium situations than it is in equilibrium.

[1] J. K. Freericks, H. R. Krishnamurthy and Th. Pruschke, Phys. Rev. Lett. 102, 136401 (2009). 10.1103/PhysRevLett.102.136401

[2] J. K. Freericks, H. R. Krishnamurthy, Yizhi Ge, A. Y. Liu, and Th. Pruschke, phys. stat. sol. b 246, 948–954 (2009). 10.1002/pssb.200881555

[3] B. Moritz, T. P. Devereaux, and J. K. Freericks, Phys. Rev. B 81, 165112 (2010). 10.1103/PhysRevB.81.165112

[4] B. Moritz, T. P. Devereaux, and J. K. Freericks, Comp. Phys. Commun. 182, 109 (2011). 10.1016/j.cpc.2010.05.020.