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Time-dependent Liouville density functional theory for laser-induced ultrafast demagnetization in ferromagnets[1] GUOPING ZHANG, Department of Physics, Indiana State University, Terre Haute, IN 47809, USA, YI-HUA BAI, Office of Information Technology, THOMAS F GEORGE, University of Missouri-St. Louis — Abstract: The traditional time-dependent density functional theory is very powerful to simulate the dynamic process, but is very time consuming. When it was first used to understand laser-induced ultrafast demagnetization in ferromagnets, the results were disappointing, with the laser amplitude at least three orders of magnitude larger than the experimental one to achieve the similar spin reduction. We develop a new theory within the density functional theory (DFT) for laser-induced ultrafast demagnetization in ferromagnets. We first solve the Liouville equation in the time domain and then feed the excited state density into the DFT code, so the dynamics proceeds on the excited and constraint potential surface. We test this for several magnetic systems and find a significantly larger demagnetization than the static approach, but is still smaller than the experimental finding. Both the local density approximation and the generalized gradient approximation fail. Our finding strongly suggests that a new functional must be developed. As a first test, we introduce a spin power scaling method. Some primitive results will be presented.

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