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Kinetic Density Functional Theory for Plasmonic Nanostructures
LUCAS V. BESTEIRO, Ohio University, HUI ZHANG, Rice University, ALEXANDER GOVOROV, Ohio University — We present a quantum kinetic theory of the dynamic response of typical noble metals [1]. The kinetic DFT is derived starting from the master equation of motion for the density matrix, which involves both momentum and energy relaxation processes. Therefore, the quantum system is described by two relaxation parameters, unlike the conventional time-dependent DFT incorporating only one relaxation parameter. This allows us to describe both the absorption of light and the generation of hot plasmonic electrons. The proposed theory can be employed to model and predict a variety of metal and hybrid nanostructures for applications in photocatalysis, sensors, photodetectors, metamaterials, etc. To support this, we show how the formalism can provide insights on several recent experimental results [2-4]. [1] A.O. Govorov, H. Zhang, J. Phys. Chem. C 119, 6181 (2015). [2] L. Weng, H. Zhang, A. O. Govorov, and M. Ouyang, Nature Commun. 5, 4792 (2014). [3] H. Harutyunyan, A.B.F Martinson, D. Rosenmann, L.K. Khorashad, L.V. Besteiro, A.O. Govorov, G.P. Wiederrecht, Nature Nanotech. 10, 770 (2015). [4] W. Li, Z.J. Coppens, L.V. Besteiro, W. Wang, A.O. Govorov, J. Valentine, Nat. Commun. 6, 8379 (2015).

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