

Abstract Submitted  
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**Is the Kohn-Sham Oscillator Strength Exact at the Ionization Threshold?**<sup>1</sup> ZENGHUI YANG, University of California, Irvine, CA 92697, USA, META VAN FAASSEN, Afdeling Theoretische Chemie, Vrije Universiteit, De Boelelaan 1083, 1081 HV Amsterdam, Kingdom of the Netherlands, KIERON BURKE, University of California, Irvine, CA 92697, USA — It is well-established that the highest occupied orbital of the exact Kohn-Sham potential of any system is at  $-I$ , where  $I$  is the ionization energy. Therefore, in optical response, the non-interacting Kohn-Sham electrons in the ground-state potential have a first ionization threshold that exactly matches that of the real system[1]. We show that corresponding the Kohn-Sham oscillator strength is not exact at the first ionization threshold by explicit demonstration for the helium atom. We use a simple fit of the entire photoabsorption spectrum of both the Kohn-Sham potential for helium and that of real helium. We use oscillator strength sum rules[2] to determine the fit parameters, so this fit should be generally useful. [1] M. A. L. Marques, C. A. Ullrich, F. Nogueira, et al. Time-Dependent Density Functional Theory. Springer-Verlag, Berlin, 2006 [2] U. Fano and J. W. Cooper. Rev. Mod. Phys., 40(3), 441-507, 1968

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