Title:	Rotatory Response of Molecular Electron Momentum Densities in Linear, Homogeneous Weak Electric Fields: A Topographical Analysis
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Abstract:	One-electron properties for molecules such as electron density, electrostatic potential (ESP), and electron momentum density (EMD) are experimentally tractable quantities, useful in understanding chemical characteristics. In this work, effects of a uniform homogeneous external electric field on some characteristic one-electron properties of simple molecules are analyzed. EMDs and ESPs were used to understand the response of water, hydrogen fluoride, carbon monoxide, chloroacetylene, and ammonia in an electric field. Remarkably, the EMD maxima for these molecules get rotated as the electric field strength is varied. A greater order of change in EMD than in ESP with increasing electric field strength brings out the sensitivity of the EMDs, especially for the valence electronic region, which in the momentum space is mapped onto the vicinity of its origin. The eigenvectors of the EMD Hessian maxima at the momentum-space origin are seen to rotate as a function of increasing field strength, with the extra angular momentum imparted by the field manifesting itself as reconfiguration of the EMD distribution. In the presence of the field, valence states may couple with higher electronic states, leading to a mixing of the states resulting in avoided crossings as a function of the field strength. The avoided crossings legitimately estimate maximal field strength limits for the calculation, prior to ionization.
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