Deep Learning and Retrieval Internuclear Distance in a Molecule From Holographic Interference Patterns

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Strong-field photoelectron holography (SFPH) is a rapidly developing method for visualization of electronic and molecular dynamics in real-time [1]. In the SFPH, the hologram is created by the interference of the rescattered electrons that are driven back to their parent ions and rescatter on them with direct electrons that do not rescatter. Although significant progress has been made recently in the investigations of the SFPH, the effects of the nuclear motion in a molecule on the holographic patterns (see [2]) require further studies. Such studies, in turn, require an analysis of the changes in the holographic patterns with varying the internuclear distance when nuclei are treated as frozen during the interaction with the laser pulse. However, the quantification of these changes is a nontrivial task.

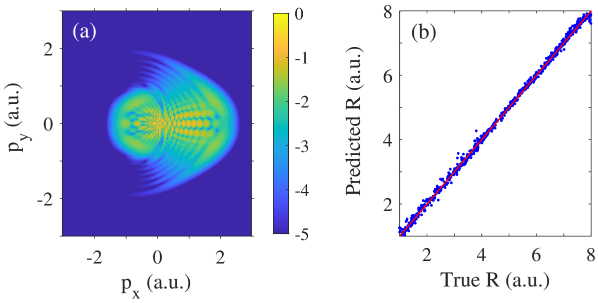

Figure 1: (a) Photoelectron momentum distribution for ionization of the two-dimensional H_2^+ molecule with the internuclear distance $R = 2.0$ a.u. by a laser pulse with a duration of 2 optical cycles, the wavelength of 800 nm, and intensity of 4.0×10^{14} W/cm^2. (b) The plot of the predicted vs. true internuclear distance demonstrating the performance of the neural network

We train and apply a convolutional neural network (CNN) to predict the internuclear distance in the H_2^+ molecule based on the momentum distributions of the photoelectrons ionized by a strong laser pulse [3]. The photoelectron momentum distributions are calculated from the direct numerical solution of the two-dimensional time-dependent Schrödinger equation. We show that the CNN trained on a dataset consisting of only a few thousand images can efficiently predict the internuclear distance with the mean absolute error of about 0.1 a.u. (see Fig. 1). Furthermore, we study the effect of focal averaging on the retrieval of the internuclear distance. The CNN trained on the set of focal averaged electron momentum distributions shows an excellent performance providing the mean absolute error less than 0.2 a.u. The obtained results will be used as a necessary benchmark for further developments of the SFPH technique.

References

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