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High-performance simulations of high-order harmonic generation based on artificial intelligence

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Artificial intelligence is an emerging field that is being successfully used in a broad set of fields and applications, including physics. Thanks to the growing computing power provided by modern GPUs —and software libraries that allows to easily use these technologies—, artificial intelligence (and particularly deep learning) is becoming a powerful tool in ultrafast and nonlinear optics. For example, machine learning algorithms can predict the X-ray pulse properties of free electron lasers [1].

One of the fields in which artificial intelligence may provide powerful computing capabilities is in the simulation of high-order harmonic generation (HHG). HHG is a nonperturbative process in which high-order harmonics— extending up to the X-rays— result from the highly nonlinear interaction of an intense, infrared femtosecond laser pulse, with an atomic, molecular or solid target. The exact simulation of HHG requires a detailed evolution of the electronic wavepacket dynamics in the vicinity of each atom or molecule of the target, which is obtained through the resolution of the time-dependent Schrödinger equation (TDSE). Solving TDSE for single-atom HHG simulations using modern hardware is quite time consuming. However, a simulation that can be compared to experiments requires its macroscopic description, i.e. to account for the harmonic emission in all the atoms in the target. Thus, the macroscopic simulation would require to solve the TDSE 10^3 to 10^6 times, which makes the macroscopic simulation prohibitive. Our group has expertise in the development of microscopic and macroscopic approaches to simulate HHG in the most stringent situations [2, and citations therein]. Interestingly, it has been recently proposed to use deep neural networks to speed-up the microscopic TDSE calculation in HHG [3].

In this work we propose to apply artificial intelligence to macroscopic simulations of HHG. We create and train a neural network to infer single-atom HHG calculated through the TDSE (see Fig. 1), so macroscopic calculations can take advantage of this trained network to obtain experimentally comparable results of TDSE. This improvement will allow us not only to accelerate the macroscopic simulations of HHG, but to obtain for the first time TDSE-based macroscopic simulations of HHG, without the need of resorting to approximations like the Strong Field Approximation. As a consequence, studies of the macroscopic signature of effects that are not well reproduced in such approximations, like electronic correlations or the properties of low-order, perturbative harmonics, can be theoretically studied. In addition, we belive that artificial intelligence can set the path towards in-situ simulations that can guide future HHG experiments.

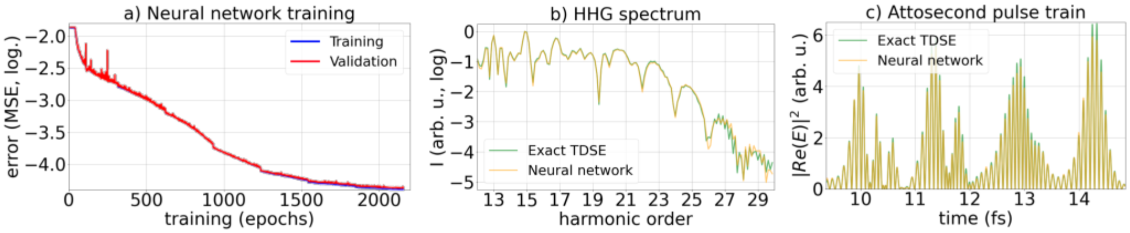

Figure 1. a) Evolution of the error (MSE) of the neural network during training with the TDSE. Sample single-atom results in the frequency (b) and time (c) domain using TDSE (green) and the neural network (orange).

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[3] Lytova, M., Spanner, M. et al. Deep learning and high harmonic generation, *arXiv:2012.10328v2* (2021)

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