Ehrenfest's theorem and the validity of the two-step model for strong-field ionization

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Semiclassical models applying a classical description of the electron after it has been promoted into the continuum by tunneling are now widely used in strong-field physics. The investigation of the applicability region of such approaches is particularly important in view of the rapid progress in experimental techniques, which has made it possible to study strong-field processes in completely new and unexplored regions of laser parameters. We have addressed the question about the applicability of the two-step semiclassical model [1, 2] of ionization by strong laser fields [3]. Our analysis is based on a quantitative comparison of the results obtained by the two-step model with the exact solution of the time-dependent Schrödinger equation (TDSE).

We have found [3] a correlation between the invalidity of the two-step model and the deviation from what we define as the «strict» form of the Ehrenfest's theorem (ET) for an ensemble of classical trajectories:

$$\frac{d\langle \boldsymbol{r}\rangle}{dt}=\langle \boldsymbol{p}\rangle,\ \ \frac{d\langle \boldsymbol{p}\rangle}{dt}=-\nabla_{\boldsymbol{r}}V(\boldsymbol{r},t)\Big|_{\boldsymbol{r}=\langle \boldsymbol{r}\rangle}.$$

Here $\langle \boldsymbol{r}\rangle$ and $\langle \boldsymbol{p}\rangle$ are average position and momentum, respectively, and $V(\boldsymbol{r},t)$ is the potential. We have introduced a measure for the deviation from the strict form of the ET, i.e., the relative deviation between the force at the average position of the classical ensemble and the average of the force. We showed that even substantial deviations from the strict form of ET at times close the electron ejection, as well as at the end of the pulse, do not affect the agreement between the solution of the TDSE and the two-step model. However, a substantial deviation from the strict form of ET at any other time should be considered as a manifestation of inapplicability of the two-step model, at least for an adequate description of the momentum distributions. We have calculated the maximal relative deviations and the times of these deviations as a function of the parameters of the laser pulse and of the atomic target: ellipticity, wavelength, intensity, ionization potential, and the potential range. By doing so, we have explored the trends of the applicability of the two-step semiclassical model.

In addition to H, we investigated the applicability of the two-step model for the following atomic targets: Mg, Xe, Kr, Ar, Ne, and He, taking into account the corresponding Stark shifts of the initial states and polarization-induced dipole potentials. The results of this study can be used as a guideline for the applicability of the two-step semiclassical model for strong-field ionization, depending on the parameters of the laser pulse and the target atom.

References:

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