# 3E04 Phase space approach to intense-laser-driven electronic wavepacket propagation

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We propose a new method to solve the time-dependent Schrödinger equation based on a phase space perspective [1]. The method employs the periodic von Neumann basis with biorthogonal exchange (pvb basis) recently introduced for the calculation of the energy eigenstates of time-independent quantum systems [2]. While the individual elements in this basis set are time-independent, a small subset is chosen in a time-dependent manner to adapt to the evolution of the wavepacket in phase space. The resulting method is simple, efficient, accurate, flexible, and stable. Our long-term goal is to apply the method to simulate the correlated dynamics of multiple electrons in atoms and molecules in intense and ultrashort laser pulses. As a first demonstration, we present calculations of electron dynamics in a 1D model atom interacting with the combined field of intense near-infrared (NIR) and attosecond extreme-ultraviolet (XUV) laser pulses.

In Fig. 1, we show the simulated evolution of the 1D electronic wavepacket in phase space. The NIR laser pulse ($5 \times 10^{13}$ W/cm$^2$, 800 nm, 4 fs) and the XUV laser pulse ($1 \times 10^{12}$ W/cm$^2$, 15 nm, 250 as) were applied to the electron in a 1D soft-core Coulomb potential. In the pvb basis, the expansion coefficients of a wavepacket are given by the projection of the wavepacket to phase space Gaussians imposed with periodic boundary conditions. Squared moduli of these coefficients are shown by the red color scale on the ellipses, which have the same center and aspect ratio as the corresponding phase space Gaussians. A lattice of $64 \times 64$ Gaussians is required to span the rectangular boundary of each panel in Fig. 1, but only those Gaussians indicated by the ellipses have significant overlap with the wavepacket. The active Gaussians are predetermined by running classical trajectories for a simplified model. The representation with the full set of Gaussians is equivalent to the representation using the same number of Fourier grid points. However, the localized nature of the Gaussians allowed us to propagate the wavepacket using only about 10 % of the pvb basis with negligible loss of accuracy.

Figure 2 shows the photoelectron momentum distribution that emerges from the simulation in Fig. 1 (blue solid line). Comparison with a simulation using the full pvb basis (red dashed line) indicates that the small active set not only reproduces the qualitative features, such as the direct (N1 and N1') and rescattered (N2 and N2') NIR-photoelectron cut-offs as well as the NIR-streaked single-XUV-photon ionization peaks (X1 and X1'), but also has quantitative accuracy.

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[1] N. Takemoto, A. Shimshovitz, and D.J. Tannor, J. Chem. Phys. **137**, 011102 (2012).
[2] A. Shimshovitz and D.J. Tannor, Phys. Rev. Lett. (in press) [e-print arXiv:1201.2299v1].

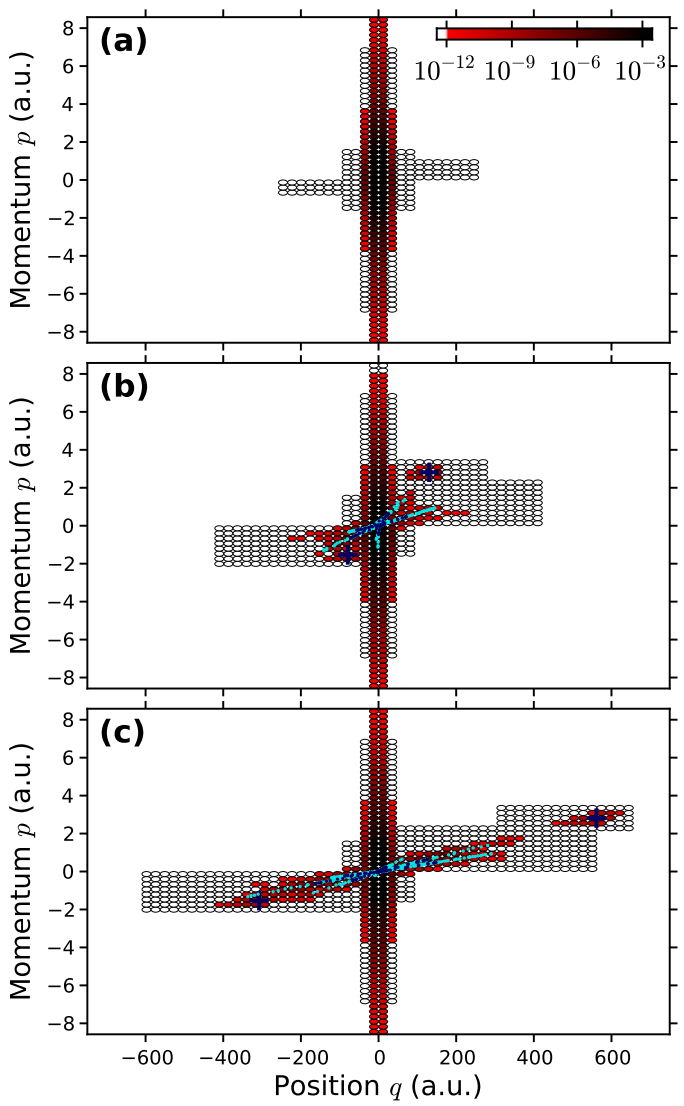


FIG. 1. Snapshots of the wavepacket in phase space. The squared moduli of the overlaps of the wavepacket to the phase space Gaussians are shown by the red color scale. The dark- and light-blue dots as well as dark-blue + marks represent the classical trajectories used to predetermine which Gaussians will have significant overlap.

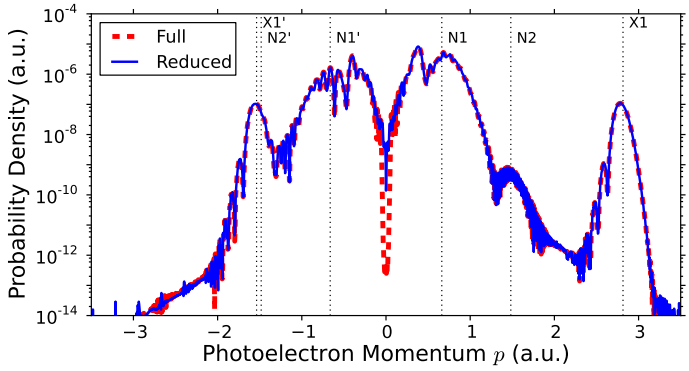


FIG. 2. Photoelectron momentum distribution. The results with the reduced (blue solid line) and full (red dashed line) pvb bases are compared.