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Multiple-Scattering Phase Distortion in the Ionization of Molecules

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Synopsis We theoretically analyze the multiple-scattering effects that might occur in the ionization of a molecule by the impact of photons or massive particles, by calculating the series to all orders within a muffin-tin description. We find a large sensitivity on the final state and a sizable momentum-dependent distortion of the phase-shift and frequency of the interference oscillations, that are not replicated by non-scattering or single-scattering approximations. Furthermore, our results do not validate the existence of any discernible harmonic oscillations.

In 1966, Cohen and Fano [1] predicted the appearance of interferences in the photoionization of molecules, a simple effect that was experimentally confirmed not only for photon impact, but also for electrons, protons and ions colliding with different molecular targets.

Since these interference effects are intrinsic to the non-local coherence of the initial bound state, even a simple linear combination of initial atomic orbitals and a plane-wave final state are enough to explain them [1]. In fact, simple non-scattering calculations show a fair agreement with the experimental results. However, the emitted electron does not move freely but in the presence of other atomic partners, whose multicenter geometry might be behind some deviations displayed by the experimental data [2, 3, 4]. Single-scattering processes were incorporated in order to tackle these problems [3, 5], but did not suffice to explain all the observed discrepancies [4, 6].

In order to shed light on the origin of these deviations, we calculate the full Multiple-Scattering series to all orders within a muffin-tin description. We demonstrate that the simple Debye-Ehrenfest formula of non-scattering models is recovered for large values of the emitted electron momentum transfer. However, our description presents a large sensitivity on the final state and differs significantly from non-scattering and single-scattering models for small and intermediate momentum transfers. Actually, we demonstrate that multiple-scattering effects produce a sizable distortion of the oscillations. In particular, the phase-shift and frequency distortions are shown to be momentum dependent, a fact that might explain why the use of a constant shift and / or a uniform modification of the frequency failed to provide a fair fitting of the experimental data [2].

Finally, our results do not validate the existence of any discernible harmonic oscillations as those claimed to have been experimentally observed [2], indicating that multiple-scattering effects should be acting in a more subtle way than assumed so far.

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