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Theoretical study on laser-assisted electron momentum spectroscopy of helium

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Introduction and motivation

Almost a half-century ago Smirnov and Neudatchin proposed to use the $(e, 2e)$ method at high impact energy and large momentum transfer for measurement of electron momentum distribution in matter [1]. Since then it has developed into a powerful tool for exploring the electronic structure of various systems, ranging from atoms and molecules to clusters and solids. In the literature it is often referred to as *electron momentum spectroscopy (EMS)* (see Refs. [2, 3] and references therein).

The impressive advance in laser technologies stimulated a notable growth of interest to laser-assisted atomic collisions in last decades. In particular, Höhr et al. [4] recently carried out the first kinematically complete $(e, 2e)$ measurements on He in the presence of laser radiation. This indicates that the first laser-assisted EMS measurements are feasible in the near future. The corresponding theoretical studies have appeared only very recently [5]. At the present stage, the main task of the theory is to analyze the potential of the EMS method for investigating laser-modified momentum distributions of electrons in matter. The analysis [5] was carried out for atomic hydrogen, which is a benchmark system for EMS. However, from the viewpoint of experimental realization, a helium atomic target seems to be more convenient and “easy-to-use”. Therefore, we study theoretically the laser-assisted EMS of helium, mainly focusing on ionization-excitation processes (clearly, such processes are absent in the hydrogen case). In this contribution we report on the pilot calculations, which can be useful in planning and preparation of the corresponding experiments.

EMS in the field-free case

The key feature of EMS is the kinematics of quasielastic knockout of the target electron by the fast incoming electron at large energy and momentum transfer. This is realized under the so-called high-energy Bethe ridge conditions, when the energy and momentum transferred to the target are absorbed by the ejected electron.

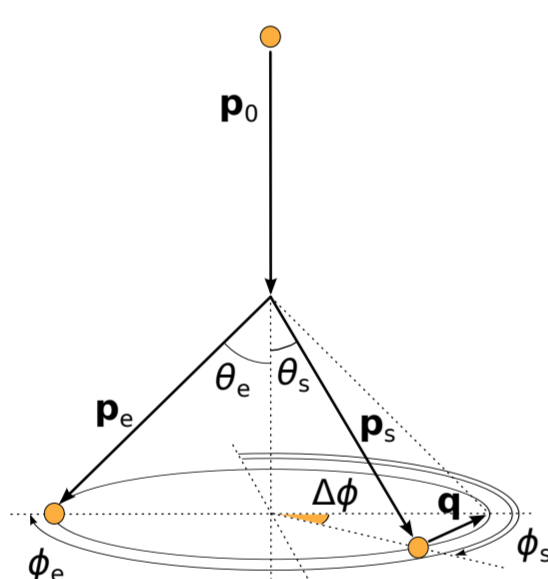


Figure 1: A sketch of the $(e, 2e)$ process in noncoplanar geometry.

A typical EMS setup assumes symmetric noncoplanar geometry (see Fig. 1) such that

$$E_s = E_e \simeq E_0/2, \quad \theta_s = \theta_e = \pi/4.$$

The coincident differential cross section of the process is measured as a function of the recoil-ion momentum

$$\mathbf{q} = \mathbf{p}_0 - \mathbf{p}_s - \mathbf{p}_e.$$

The absolute value of \mathbf{q} is given by

$$q = \sqrt{(p_0 - \sqrt{2}p_s)^2 + \left(\sqrt{2}p_s \sin \frac{\Delta\phi}{2}\right)^2}.$$

Describing the fast incoming and outgoing electrons by plane waves and involving the Born approximation, one obtains the fully differential cross section (FDCS) as

$$\frac{d\sigma}{dE_e dE_s d\Omega_s d\Omega_e} \propto |\psi(\mathbf{q})|^2, \quad (1)$$

where $|\psi(\mathbf{q})|^2$ is the one-electron momentum density of the ionized electron orbital. The shape of the FDSC as a function of kinematical variables depends strongly only on q and therefore it is usually called the momentum profile [3].

Theory of laser-assisted EMS

We consider the case of a linearly polarized laser wave with frequency ω and a wave vector \mathbf{k} ($k = \omega/c$). A typical situation is when the laser wavelength $\lambda = 2\pi/k$ is much greater than the spatial extent both of the target and of the region where the electron-electron collision takes place. This validates the use of the dipole approximation for the electric component and vector potential of the laser field, respectively,

$$\mathbf{F}(t) = \mathbf{F}_0 \cos \omega t, \quad \mathbf{A}(t) = -\frac{c}{\omega} \mathbf{F}_0 \sin \omega t.$$

Theory of laser-assisted EMS

In order to minimize possible photoionization effects, the electric-field amplitude F_0 and the field frequency ω are supposed to be small on the atomic scale.

In what follows, we consider two different orientations of the polarization plane, which are depicted in Fig. 2. The first one (LP \parallel) is when the electric-field direction coincides with that of \mathbf{p}_0 and the second one (LP \perp) when it is perpendicular to the scattering plane.

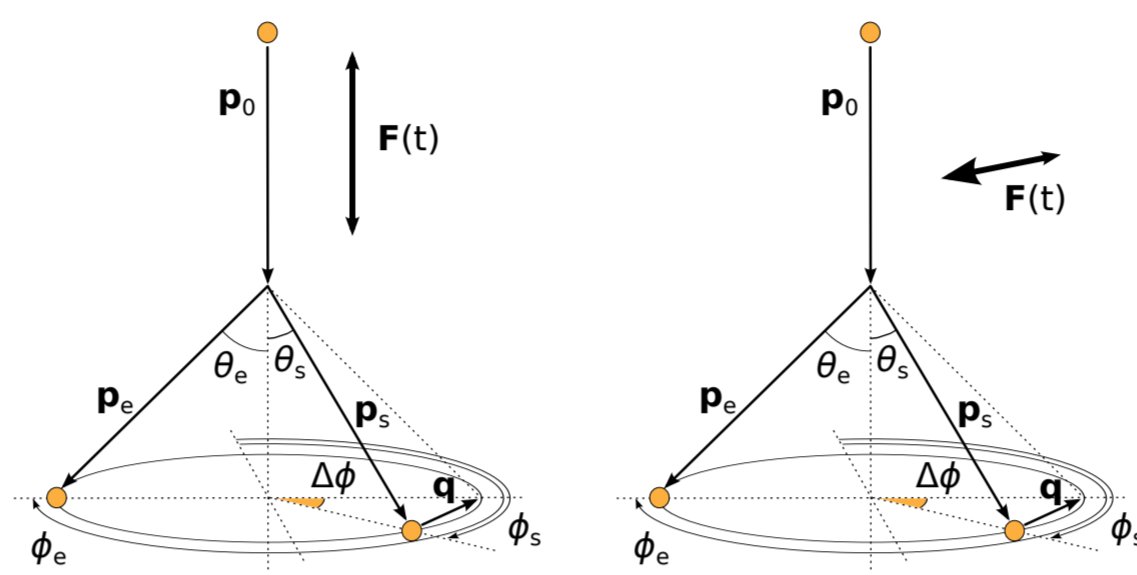


Figure 2: LP \parallel (left) and LP \perp (right) geometries of the laser-assisted EMS process.

Using the Born and binary-encounter approximations, the S -matrix for the laser-assisted EMS process is evaluated as

$$S = -i \int_{-\infty}^{\infty} dt \langle \chi_{p_s}(t) \chi_{p_e}(t) \psi_f(t) | v_{ee} | \chi_{p_0}(t) \psi_i(t) \rangle,$$

where χ_p stands for the incoming and/or outgoing electron wave, $\psi_{i,f}$ are the initial atomic and the final ionic states, respectively, and v_{ee} is the Coulomb potential between the colliding electrons.

The incoming and outgoing electron states are described using Volkov functions, which are solutions to the Schrodinger equation for the electron motion in a plane electromagnetic wave, that is

$$\chi_p(\mathbf{r}, t) = \exp\{i[\mathbf{p}\mathbf{r} - \gamma \sin \omega t - Et - \zeta(t)]\}, \quad (2)$$

where

$$E = \frac{p^2}{2}, \quad \gamma = \frac{\mathbf{p}\mathbf{F}_0}{\omega^2}, \quad \zeta(t) = \frac{1}{2c^2} \int_{-\infty}^t A^2(t') dt'.$$

If one neglects the laser-field effects on the incoming and outgoing electrons, then the Volkov function (2) reduces to a usual plane wave,

$$\chi_p(\mathbf{r}, t) = \exp[i(\mathbf{p}\mathbf{r} - Et)]. \quad (3)$$

In Ref. [6], the plane-wave and Volkov-function treatments were compared and the latter was shown to be necessary to obtain the correct shape of the momentum profile.

It can be shown that the FDSC has a form of a sum over processes with different number of emitted ($N > 0$) or absorbed ($N < 0$) photons:

$$\frac{d\sigma}{dE_s dE_e d\Omega_s d\Omega_e} = \sum_{N=-\infty}^{\infty} d^3\sigma_N \delta(E_s + E_e + \mathcal{E}_f - E_0 - \mathcal{E}_i + N\omega),$$

where the N -photon triple differential cross section (TDCS) is given by

$$d^3\sigma_N = \frac{p_s p_e}{(2\pi)^3 p_0} \left(\frac{d\sigma}{d\Omega} \right)_{ee} |\mathcal{F}_N(\mathbf{q})|^2, \quad (4)$$

with $(d\sigma/d\Omega)_{ee}$ being the half-off-shell Mott-scattering cross section that takes account of exchange between the colliding electrons, and \mathcal{F}_N is the momentum profile assisted by the N -photon process.

Numerical results

We performed numerical calculations of the TDCS (4) with the following parameters:

$$\text{Laser field intensity: } I = 4 \cdot 10^{12} \text{ W/cm}^2$$

$$\text{Laser field frequency: } \omega = 1.17 \text{ eV}$$

$$\text{Incident electron energy: } E_0 = 2000 \text{ eV} - \mathcal{E}_i$$

The above laser parameters are the same as those of the Nd:YAG laser utilized in the first laser-assisted $(e, 2e)$ experiments [4].

Three different ground-state wave functions of He were considered: Roothaan-Hartree-Fock (RHF), Silverman-Platas-Matsen (SPM), and Bonham-Kohl (BK). RHF treats electrons as noninteracting particles moving in a mean-field spherically symmetric potential, SPM takes into account radial correlation between the electrons, and BK accounts for both radial and angular correlations. Since the discussed electromagnetic field is weak, its effect on the initial atomic and final ionic states, ψ_i and ψ_f , can be described using perturbation theory.

Numerical results

The results when the He⁺ ion remains in the ground state (1s) are shown in Fig. 3. Strong dependence of the momentum profiles on the field orientation is observed (compare the cases of LP \parallel and LP \perp geometries).

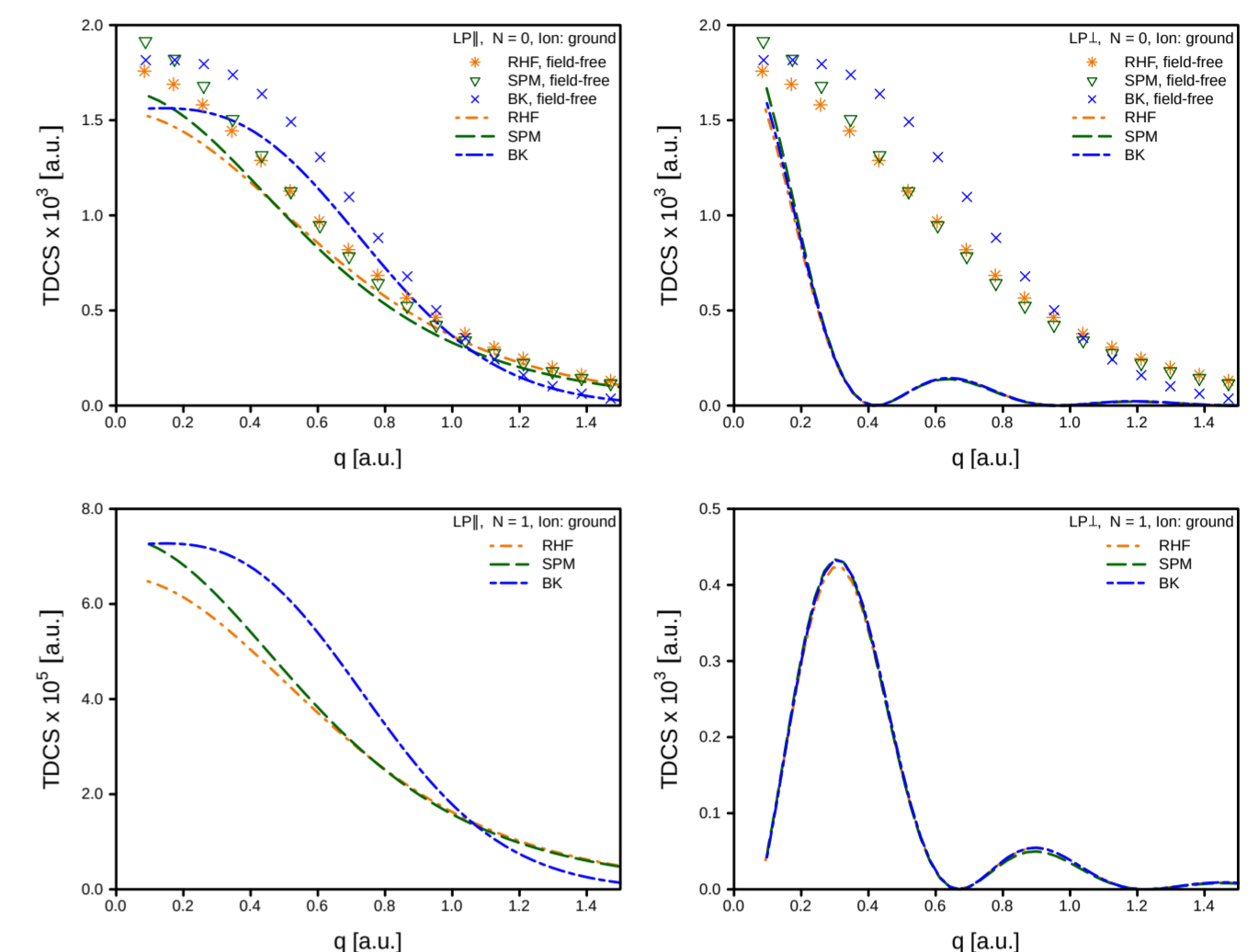


Figure 3: The $N = 0, 1$ TDCS in the case of transition to the ground state of the He⁺ ion. The LP \parallel (left) and LP \perp (right) geometries are specified in Fig. 2.

The EMS process involving excitation of the residual ion is a powerful tool for studying electron correlations in a target. Since the electron ejection from helium takes place due to knockout, which is a first-order mechanism, excitation of the He⁺ ion can be realized only via the shakeup mechanism. The latter is governed by electron correlations.

The first excited state of the He⁺ ion is fourfold degenerate (2s and 2p $_{0,\pm 1}$ orbitals). We sum the corresponding cross sections because these orbitals are not resolved in experiment. The results are presented in Fig. 4. Note that the uncorrelated, RHF function gives significantly different results both in the field-free and in the laser-assisted cases.

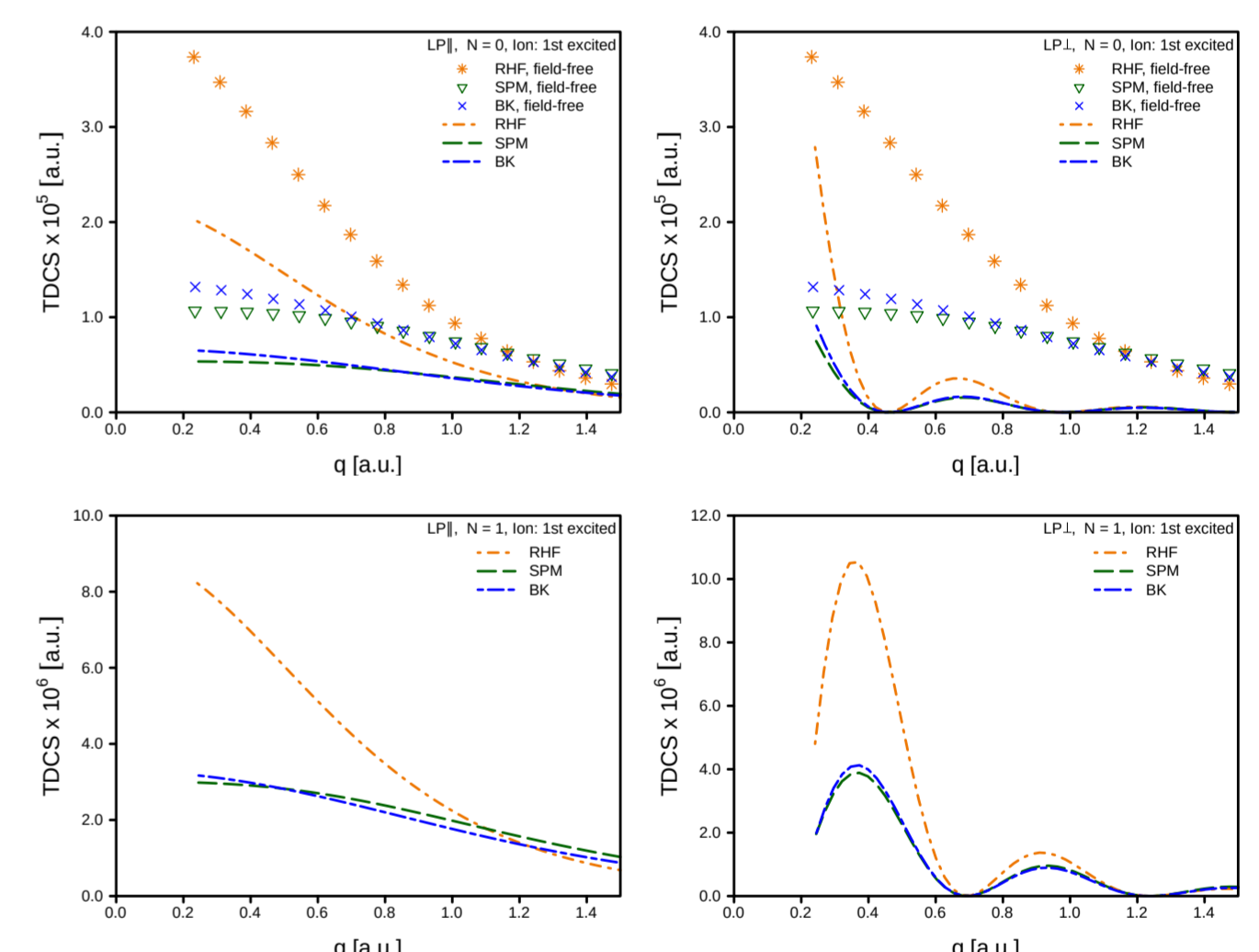


Figure 4: The same as in Fig. 3 but when the He⁺ ion is in the first excited state.

Conclusions

On the basis of the presented numerical results, the following conclusions can be made:

- ▶ Even at small field strengths ($F_0 \sim 10^{-2}$ a.u.), the momentum profiles strongly depend on the orientation of the laser field.
- ▶ The momentum profiles are highly sensitive to the employed helium functions.

To summarize, further theoretical analysis is desirable in order to shade more light on the potential of the laser-assisted EMS for studying laser effects on electron momentum distributions in atoms. The presented pilot numerical results can serve as a reference point for the corresponding experiments, which are planned or under way.

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