

Electron-molecule scattering in a strong laser field: Two-center interference effectsJ. Dakić,¹ D. Habibović,¹ A. Čerkić,¹ M. Busuladžić,^{2,1} and D. B. Milošević^{1,3,4}¹*Faculty of Science, University of Sarajevo, Zmaja od Bosne 35, 71000 Sarajevo, Bosnia and Herzegovina*²*Faculty of Medicine, University of Sarajevo, Čekaluša 90, 71000 Sarajevo, Bosnia and Herzegovina*³*Academy of Sciences and Arts of Bosnia and Herzegovina, Bistrik 7, 71000 Sarajevo, Bosnia and Herzegovina*⁴*Max-Born-Institut, Max-Born-Strasse 2a, 12489 Berlin, Germany*

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Laser-assisted scattering of electrons on diatomic molecules is considered using the S -matrix theory within the second Born approximation. The first term of the expansion in powers of the scattering potential corresponds to the direct or single laser-assisted scattering of electrons on molecular targets, while the second term of this expansion corresponds to the laser-assisted rescattering or double scattering. The rescattered electrons may have considerably higher energies in the final state than those that scattered only once. For multicenter polyatomic molecules scattering and rescattering may happen at any center and in any order. All these cases contribute to the scattering amplitude and the interference of different contributions leads to an increase or a decrease of the differential cross section in particular electron energy regions. For diatomic molecules there are two such contributions for single scattering and four contributions for double scattering. Analyzing the spectra of the scattered electrons, we find two interesting effects. For certain molecular orientations, the plateaus in the electron energy spectrum, characteristic of laser-assisted electron-atom scattering, are replaced by a sequence of gradually declining maxima, caused by the two-center interference effects. The second effect is the appearance of symmetric U-shaped structures in the angle-resolved energy spectra, which are described very well by the analytical formulas we provide.

DOI: [10.1103/PhysRevA.96.043406](https://doi.org/10.1103/PhysRevA.96.043406)**I. INTRODUCTION**

Nonlinear atomic and molecular processes in a strong laser field have attracted a great deal of attention in the past few decades due to numerous applications in chemistry, physics, and biology. All these processes can be categorized into two main classes. One consists of laser-induced processes that are possible only in the presence of a strong laser field. Some of the most investigated phenomena from this class are high-order-harmonic generation (HHG) and high-order above-threshold ionization (HATI) (see review articles [1,2] and references therein). In the first step of these processes, the considered atomic or molecular system absorbs more photons from the laser field than is necessary for ionization [3]. The electron, freed in such a way, can go directly to the detector. We call this process direct above-threshold ionization (ATI). Due to the influence of the laser field, the ionized electron may also return to the parent molecular ion (second step) and elastically scatter on it (third step), before reaching the detector. In this process, the electron can absorb many more photons from the laser field than in direct ATI. This process is called high-order ATI (in the case of atomic targets see [4]). In the third step of the HHG process, the electron recombines with the parent ion and a high-energy photon is emitted [5,6]. The energy spectra of molecular HATI and molecular HHG processes are characterized by a plateau that manifests itself as a broad energy interval of the spectrum in which the photoelectron (HATI) or photon (HHG) yield is practically constant.

There are also processes that can occur without the influence of the laser field, such as the laser-assisted electron-ion radiative recombination (LAR) and the laser-assisted electron-atom or -molecule scattering (LAS). The laser-assisted electron-atom potential scattering in the first Born approximation was first analyzed by Bunkin and Fedorov [7] (for better insight and a deeper understanding of the laser-assisted processes, see

[8,9] and references therein). Our aim is to present a theoretical approach by which one can describe and analyze in detail the laser-assisted electron-molecule scattering. Although the laser-assisted processes can occur in the absence of the laser field, they are modified by the simultaneous interaction with the laser radiation. In other words, structures obtained in photon and electron spectra are enriched by the interaction with the laser field. For example, in LAR [10–12], LAS [13–18], and laser-assisted x-ray-atom scattering [19,20], the emitted photon and electron spectra exhibit a long plateau that is followed by an abrupt cutoff. Such a plateau is formed due to the absorption of a large number of laser photons.

Molecules are multicenter systems. Therefore, additional multicenter interference effects appear in the above-mentioned third step and by analyzing the electron (photon) spectra we can obtain information about the molecular structure and symmetry. In fact, even the direct ionization without rescattering reveals the initial symmetry of the molecular system. For example, the O_2 molecule shows a suppression in the low-energy part of the electron spectrum, due to its π_g symmetry, while the N_2 molecule, having σ_g symmetry, does not show such a suppression [21–25].

In the rescattering process, for diatomic molecules, there are four contributions to the ionization rate, which are responsible for the high-energy plateau in the electron (photon) spectra and interfere in a complicated manner [26,27]. The spectra are even more complicated due to the different symmetry properties of the atomic orbitals of which a particular molecular orbital consists. By analyzing these spectra for different angles between the molecular axis and the laser polarization axis, and for different electron emission angles with respect to the laser polarization axis, one can obtain information about molecular symmetry. The ionization, as well as the rescattering, can happen at different centers, producing interference structures

in the electron spectrum [28,29]. This type of interference survives the focal averaging and even has been observed in the HATI experiment with unaligned molecules [30]. The double-slit-type or two-point emitter interference in HHG also manifests itself as a series of minima and maxima in the harmonic yield for particular values of the angle between the internuclear axis and the laser polarization axis, which is accompanied by a jump of the harmonic phase by π [31]. In Ref. [32] laser-induced backscattering holography was used to probe the molecular dynamics.

All the above-cited papers have been mostly devoted to the nonlinear processes with homonuclear diatomic molecules. More recently, the behavior of polar molecules in a strong laser field has attracted more attention. We considered HATI of heteronuclear and polyatomic molecules by a strong laser field [33,34]. Analogously to the previous case, some features of the partial contributions and total spectrum can be related to the shape of the molecular orbital. Similar theories of HHG by heteronuclear diatomic and by more complex polyatomic molecules, exposed to an arbitrarily polarized laser field, were presented in [35,36]. An interference minima condition that is valid for arbitrary heteronuclear diatomic molecules was derived for both the HATI and the HHG spectra [33,35]. In the case of polyatomic molecules, all observed minima were also produced by the multicenter interference, but the corresponding analysis is more complex than in the case of diatomic molecules [34,36].

There are a few papers in which the laser-assisted processes on molecular targets were analyzed. Kanya and co-workers proposed a method called laser-assisted electron diffraction (LAED) [37], in which sub-10-fs temporal resolution can be achieved by using a laser-assisted elastic electron scattering process. Also, they demonstrated the feasibility of LAED by measuring the electron diffraction patterns of CCl_4 molecules during the irradiation of femtosecond laser pulses [38]. More recently, Kanya and Yamanouchi proposed a method for probing geometrical structures of isolated molecules with sub-10 fs temporal resolution [39]. The Cl_2 molecule was used as the target.

As the molecules are multicenter systems, we can expect to observe a similar interference structure in the laser-assisted processes. We hope that the investigation presented in this paper should spark experiments and theoretical investigations of the laser-assisted molecular processes. This may lead to discoveries in this field of research and improve our understanding of the laser-matter interactions.

In this paper we analyze the two-center interference effects that occur in the laser-assisted scattering of electrons on diatomic molecules. Both single and double scattering are included in the analysis. We apply an independent-atom molecular model in our analysis. This model is widely used in the literature (see, for example, [39]). It is also assumed that the target electrons are inert. Therefore, our analysis is a qualitative one. The quantum-mechanical theory based on the S -matrix formalism is given in Sec. II, while the interference minimum conditions are derived in Sec. III. The numerical results are presented in Sec. IV. A summary is given and results are summarized in Sec. V. We use the atomic system of units ($\hbar = e = m_e = 4\pi\epsilon_0 = 1$).

II. QUANTUM-MECHANICAL THEORY

The S -matrix theory of the potential scattering in a strong laser field was presented in Ref. [16], where the laser-assisted electron-atom scattering was analyzed. We first present the basic steps leading to the S -matrix element for the laser-assisted electron-atom scattering. After that, we will introduce the Jacobi coordinates in order to simulate the scattering of electrons on two-center potentials (i.e., the scattering of electrons on diatomic molecules). The S -matrix element for laser-assisted scattering of electrons on a local short-range potential $V(\mathbf{r})$ can be written in the form [40,41]

$$S_{fi} = i \lim_{\substack{t' \rightarrow \infty \\ t \rightarrow -\infty}} \langle \chi_{\mathbf{k}_f}(t') | G(t', t) | \chi_{\mathbf{k}_i}(t) \rangle, \quad (1)$$

where $G \equiv G^{(+)}$ is the total retarded time-dependent Green's operator that corresponds to the total Hamiltonian

$$H(t) = -\frac{\nabla^2}{2} + V(\mathbf{r}) + H_L(t), \quad \nabla \equiv \partial/\partial\mathbf{r}, \quad (2)$$

and $|\chi_{\mathbf{k}_j}(t)\rangle$ ($j = i, f$) are Volkov wave vectors that are the solutions of the time-dependent Schrödinger equation with the Hamiltonian $-\nabla^2/2 + H_L(t)$, with \mathbf{r} the relative electron coordinate in the center-of-mass system, i.e., the electron coordinate with respect to the scattering center. The laser-atom interaction in the length gauge and the dipole approximation is $H_L(t) = \mathbf{r} \cdot \mathbf{E}(t)$, with $\mathbf{E}(t)$ the electric field vector. The Volkov wave vectors in the length gauge are defined by

$$|\chi_{\mathbf{k}}(t)\rangle = |\mathbf{k} + \mathbf{A}(t)\rangle \exp\{-i[\mathbf{k} \cdot \boldsymbol{\alpha}(t) + \mathcal{U}(t) + E_{\mathbf{k}}t]\}, \quad (3)$$

where $\mathbf{A}(t) = -\int^t dt' \mathbf{E}(t')$ is the vector potential of the laser field, $\boldsymbol{\alpha}(t) = \int^t dt' \mathbf{A}(t')$, and

$$\mathcal{U}(t) = \int^t dt' \mathbf{A}^2(t')/2 = \mathcal{U}_1(t) + U_p t, \quad (4)$$

with U_p the ponderomotive energy and $\mathcal{U}_1(t)$ the time-periodic part of $\mathcal{U}(t)$. The electron kinetic energy is $E_{\mathbf{k}} = \mathbf{k}^2/2$ and $|\mathbf{k}\rangle$ denotes the plane-wave state $\langle \mathbf{r} | \mathbf{k} \rangle = (2\pi)^{-3/2} \exp(i\mathbf{k} \cdot \mathbf{r})$.

We expand the S -matrix element (1) into a power series with respect to the scattering potential V and keep only the first-order and second-order terms in V (the second Born approximation). The result is

$$\begin{aligned} S_{fi} = & -i \int_{-\infty}^{\infty} dt \langle \chi_{\mathbf{k}_f}(t) | V | \chi_{\mathbf{k}_i}(t) \rangle \\ & - \int_{-\infty}^{\infty} dt \int_0^{\infty} d\tau \int d^3\mathbf{q} \langle \chi_{\mathbf{k}_f}(t + \tau) | V | \chi_{\mathbf{q}}(t + \tau) \rangle \\ & \times \langle \chi_{\mathbf{q}}(t) | V | \chi_{\mathbf{k}_i}(t) \rangle, \end{aligned} \quad (5)$$

where \mathbf{q} is the intermediate electron momentum, t is the time of the first scattering, and τ is the travel time (i.e., the time between the first and the second scattering). The first term on the right-hand side of Eq. (5) describes the single scattering of an electron having the initial momentum \mathbf{k}_i and the final momentum \mathbf{k}_f . The second term on the right-hand side of Eq. (5) describes the double scattering of the electron on the potential V in the laser field. The double scattering is a three-step process. In the first step, an electron with the asymptotic initial momentum \mathbf{k}_i scatters on the target in the laser field at

time t . In the second step, the once scattered electron travels in the laser field and returns to the target at time $t + \tau$. In the third step, the electron rescatters on the target and goes to the asymptotic region with the final momentum \mathbf{k}_f . The integral over intermediate electron momenta \mathbf{q} in Eq. (5) may be solved by the saddle-point method [19,42–44]. This integral can be presented as a Taylor expansion around the saddle point $\mathbf{q} = \mathbf{k}_s$, which contains powers of $1/\tau$ multiplied by the even derivatives of the subintegral function over the intermediate electron momenta. We suppose that $\tau \gg 1$, so the zeroth-order term in the expansion is dominant and all other terms may be neglected. In this way, the S -matrix element (5) becomes

$$\begin{aligned} S_{fi} &= -i \int_{-\infty}^{\infty} dt e^{i(E_f - E_i)t} \mathcal{T}_{fi}(\omega t) \\ &= -2\pi i \sum_n \delta(E_f - E_i - n\omega) T_{fi}(n), \end{aligned} \quad (6)$$

where $E_i = \mathbf{k}_i^2/2$, $E_f = \mathbf{k}_f^2/2$, ω is the angular frequency of the laser field, and

$$\begin{aligned} \mathcal{T}_{fi}(\omega t) &= e^{i\alpha(t)(\mathbf{k}_f - \mathbf{k}_i)} \left\{ \langle \mathbf{k}_f | V | \mathbf{k}_i \rangle - i \int_0^\infty d\tau \left(\frac{2\pi}{i\tau} \right)^{3/2} \right. \\ &\quad \left. \times \langle \mathbf{k}_f | V | \mathbf{k}_s \rangle \langle \mathbf{k}_s | V | \mathbf{k}_i \rangle e^{i(\mathbf{k}_f - \mathbf{k}_s)^2 \tau / 2} \right\} \\ &= \sum_{n=-\infty}^{\infty} T_{fi}(n) e^{-in\omega t}, \end{aligned} \quad (7)$$

$$T_{fi}(n) = \int_0^T \frac{dt}{T} \mathcal{T}_{fi}(\omega t) e^{in\omega t}, \quad (8)$$

with $\mathbf{k}_s = [\alpha(t) - \alpha(t + \tau)]/\tau$ representing the stationary intermediate electron momentum and $T = 2\pi/\omega$ the laser-field period. In Eqs. (6)–(8), $T_{fi}(n)$ and $\mathcal{T}_{fi}(\omega t)$ are the T -matrix element and its Fourier transform, respectively. The δ function in Eq. (6) expresses the energy-conserving condition.

All the expressions presented so far are related to the laser-assisted electron-atom scattering. As we want to analyze the laser-assisted scattering of electrons on molecular targets, which have a multicenter structure, we will introduce the Jacobi coordinates [45]. In the case of diatomic molecules, these coordinates are [46]

$$\mathbf{R} = \mathbf{R}_B - \mathbf{R}_A, \quad (9a)$$

$$\mathbf{r} = \mathbf{r}_e - \frac{M_A \mathbf{R}_A + M_B \mathbf{R}_B}{M_A + M_B}, \quad (9b)$$

$$\mathbf{R}_{\text{c.m.}} = \frac{M_A \mathbf{R}_A + M_B \mathbf{R}_B + m_e \mathbf{r}_e}{M_A + M_B + m_e}, \quad (9c)$$

where \mathbf{R}_A , \mathbf{R}_B , and \mathbf{r}_e are the coordinates of the atomic centers A and B and of the scattering electron in an arbitrary coordinate system, respectively, while M_A , M_B , and m_e are the masses of the atoms A and B and of the scattering electron, respectively. Note that \mathbf{r} is now the electron coordinate with respect to the center of mass of the molecule. The general form of the two-center scattering potential is given by [29]

$$V^{AB}(\mathbf{r}, \mathbf{R}) = V^A(\mathbf{r}_A) + V^B(\mathbf{r}_B), \quad (10)$$

where

$$\mathbf{r}_A = \mathbf{r} - C_1 \mathbf{R}, \quad \mathbf{r}_B = \mathbf{r} - C_2 \mathbf{R}, \quad (11)$$

with $C_1 = -M_B/(M_A + M_B)$ and $C_2 = M_A/(M_A + M_B)$. It can be shown that

$$\langle \mathbf{p} | V^J(\mathbf{r}_J) | \mathbf{q} \rangle = e^{i\mathbf{K} \cdot (\mathbf{r} - \mathbf{r}_J)} V_{\mathbf{K}}^J \quad (J = A, B), \quad (12)$$

where $\mathbf{K} = \mathbf{q} - \mathbf{p}$ and

$$V_{\mathbf{K}}^J = \int \frac{d^3 \mathbf{r}}{(2\pi)^3} V^J(\mathbf{r}) e^{i\mathbf{K} \cdot \mathbf{r}} \quad (J = A, B) \quad (13)$$

is the Fourier transform of the scattering potential at the atomic center J . Using Eqs. (10)–(12), we obtain the continuum-continuum matrix element of the two-center scattering potential

$$\langle \mathbf{p} | V^{AB}(\mathbf{r}, \mathbf{R}) | \mathbf{q} \rangle = e^{iC_1 \mathbf{K} \cdot \mathbf{R}} V_{\mathbf{K}}^A + e^{iC_2 \mathbf{K} \cdot \mathbf{R}} V_{\mathbf{K}}^B. \quad (14)$$

The masses of the atomic nuclei are much greater than the mass of the electron, so the motion of the atomic nuclei can be neglected and we assume that the internuclear distance is constant. Therefore, we fix the relative nuclear coordinate \mathbf{R} to the equilibrium position \mathbf{R}_0 and calculate the matrix element (14) for $\mathbf{R} = \mathbf{R}_0$. Introducing the two-center scattering potential (10) in Eq. (7), we obtain

$$\begin{aligned} \mathcal{T}_{fi}(\omega t) &= e^{i\alpha(t)(\mathbf{k}_f - \mathbf{k}_i)} \left\{ \langle \mathbf{k}_f | V^{AB}(\mathbf{r}, \mathbf{R}_0) | \mathbf{k}_i \rangle \right. \\ &\quad \left. - i \int_0^\infty d\tau \left(\frac{2\pi}{i\tau} \right)^{3/2} \langle \mathbf{k}_f | V^{AB}(\mathbf{r}, \mathbf{R}_0) | \mathbf{k}_s \rangle \right. \\ &\quad \left. \times \langle \mathbf{k}_s | V^{AB}(\mathbf{r}, \mathbf{R}_0) | \mathbf{k}_i \rangle e^{i(\mathbf{k}_f - \mathbf{k}_s)^2 \tau / 2} \right\}, \end{aligned} \quad (15)$$

where the continuum-continuum matrix elements of the two-center scattering potential are given by Eq. (14), with $\mathbf{R} = \mathbf{R}_0$, $\mathbf{p} = \mathbf{k}_f, \mathbf{k}_s$, and $\mathbf{q} = \mathbf{k}_i, \mathbf{k}_s$. The differential cross section for scattering of an electron with the initial momentum \mathbf{k}_i on a local potential $V(\mathbf{r})$, so that the final electron momentum is \mathbf{k}_f and that n photons are exchanged with the laser field ($n > 0$ for absorption and $n < 0$ for emission), is defined by [40,41]

$$\frac{d\sigma_{fi}(n)}{d\Omega} = (2\pi)^4 \frac{k_f}{k_i} |T_{fi}(n)|^2, \quad (16)$$

where the T -matrix element $T_{fi}(n)$ is defined by Eq. (8) and $\mathcal{T}_{fi}(\omega t)$ therein is given by Eq. (15).

The scattering potential at an atomic center is modeled by the sum of the polarization potential V_P and the static potential V_S , i.e., $V = V_P + V_S$. We use the polarization potential

$$V_P(r) = -\frac{\alpha_P}{2(r^2 + d^2)^2}, \quad (17)$$

where α_P is the electrostatic dipole polarizability of the atom that can be found in [47], while the parameter d is connected with α_P and nuclear charge Z by the formula $d^4 = \alpha_P/(2Z^{1/3})$ [48]. Our static potential is modeled by the double Yukawa potential

$$V_S(r) = -\frac{Z}{H} \frac{e^{-r/D}}{r} [1 + (H - 1)e^{-Hr/D}], \quad (18)$$

where $H = DZ^{0.4}$ and the values of D for various atomic targets are given in [49].

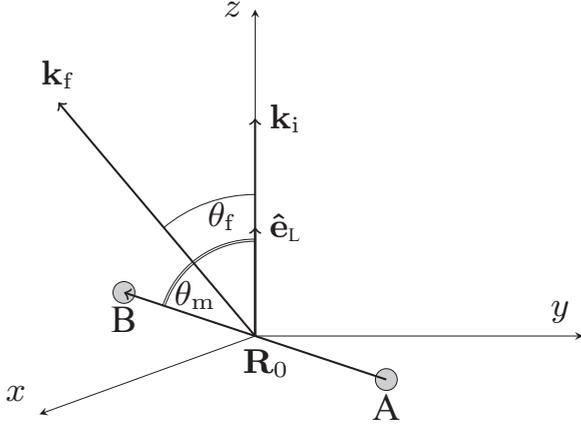


FIG. 1. Geometry of the laser-assisted electron-molecule scattering process.

We suppose that the laser field is monochromatic and linearly polarized, with the vector potential

$$\mathbf{A}(t) = \hat{\mathbf{e}}_L A_0 \cos \omega t, \quad (19)$$

where A_0 is the amplitude of the vector potential, $\hat{\mathbf{e}}_L$ is the unit polarization vector, and ω is the frequency of the laser field. In all our calculations, we assume that the unit polarization vector of the laser field $\hat{\mathbf{e}}_L$ and the incident (initial) electron momentum \mathbf{k}_i are along the z axis. The angle between the final electron momentum \mathbf{k}_f and the incident electron momentum \mathbf{k}_i is denoted by θ_f and is referred to as the scattering angle in the following. We also set $\varphi_m = 0^\circ$ for the azimuthal angle of the molecular orientation and $\varphi_f = 0^\circ$ for the azimuthal angle of the scattered electrons (i.e., the molecular axis and final electron momentum are in the xz plane). The geometry used in our calculations is presented in Fig. 1.

III. INTERFERENCE MINIMA CONDITIONS

The electron may scatter on any of the two atomic centers of the diatomic molecule, i.e., both atomic centers contribute to the scattering process. Therefore, the T -matrix element (8) and its Fourier transform (15) contain the contributions of both atomic centers to the scattering process. The destructive interference of these contributions produces the minima in the energy spectra of the laser-assisted electron-molecule scattering. In the case of homonuclear diatomic molecules, the positions of these interference minima may be determined by simple analytic methods. The interference minima condition for the single (double) scattering may be obtained from the first (second) term on the right-hand side of Eq. (15). More precisely, the part of the first (second) term that is a function of the relative nuclear coordinate $\mathbf{R} = \mathbf{R}_0$ must be set equal to zero in order to obtain the interference minima condition for the single (double) scattering.

In the case of the single scattering, we have the condition

$$e^{i(\mathbf{k}_i - \mathbf{k}_f) \cdot \mathbf{R}_0/2} + e^{-i(\mathbf{k}_i - \mathbf{k}_f) \cdot \mathbf{R}_0/2} = 0, \quad (20)$$

which may be written as

$$\cos[(\mathbf{k}_i - \mathbf{k}_f) \cdot \mathbf{R}_0/2] = 0. \quad (21)$$

Equation (21) leads to the condition

$$(\mathbf{k}_i - \mathbf{k}_f) \cdot \mathbf{R}_0 = \mp(2n_s + 1)\pi \quad (n_s = 0, 1, 2, \dots). \quad (22)$$

For $\varphi_m = \varphi_f = 0^\circ$, Eq. (22) gives

$$k_{f,n_s,\pm} = \frac{R_0 k_i \cos \theta_m \pm (2n_s + 1)\pi}{R_0 \cos(\theta_f - \theta_m)} \quad (n_s = 0, 1, 2, \dots), \quad (23)$$

where R_0 is the equilibrium internuclear distance, θ_m is the polar angle of the molecular orientation, and θ_f is the scattering angle. Therefore, the single-scattering interference minima occur at the energy values $E_{f,n_s,\pm} = k_{f,n_s,\pm}^2/2$, where $k_{f,n_s,\pm}$ is given by Eq. (23). In the case of the double scattering, we have the condition

$$\begin{aligned} & (e^{i(\mathbf{k}_s - \mathbf{k}_f) \cdot \mathbf{R}_0/2} + e^{-i(\mathbf{k}_s - \mathbf{k}_f) \cdot \mathbf{R}_0/2}) \\ & \times (e^{i(\mathbf{k}_i - \mathbf{k}_s) \cdot \mathbf{R}_0/2} + e^{-i(\mathbf{k}_i - \mathbf{k}_s) \cdot \mathbf{R}_0/2}) = 0, \end{aligned} \quad (24)$$

which is equivalent to

$$\cos[(\mathbf{k}_s - \mathbf{k}_f) \cdot \mathbf{R}_0/2] \cos[(\mathbf{k}_i - \mathbf{k}_s) \cdot \mathbf{R}_0/2] = 0. \quad (25)$$

Equation (25) leads to the conditions

$$(\mathbf{k}_s - \mathbf{k}_f) \cdot \mathbf{R}_0 = \mp(2n_d + 1)\pi, \quad (26a)$$

$$(\mathbf{k}_i - \mathbf{k}_s) \cdot \mathbf{R}_0 = \mp(2n_d + 1)\pi, \quad (26b)$$

with $n_d = 0, 1, 2, \dots$. For $\varphi_m = \varphi_f = 0^\circ$, Eq. (26a) gives

$$k_{f,n_d,\pm} = \frac{R_0 k_s \cos \theta_m \pm (2n_d + 1)\pi}{R_0 \cos(\theta_f - \theta_m)} \quad (n_d = 0, 1, 2, \dots). \quad (27)$$

The double-scattering interference minima occur at the energy values $E_{f,n_d,\pm} = k_{f,n_d,\pm}^2/2$, where $k_{f,n_d,\pm}$ is given by Eq. (27).

IV. NUMERICAL RESULTS

We will now present the energy spectra of the laser-assisted electron-molecule scattering. In all our calculations, we suppose that the laser field is defined by the vector potential (19). The assumed geometry of the scattering process is explained and illustrated at the end of Sec. II (see Fig. 1). As mentioned at the end of Sec. I, we use an independent-atom molecular model and assume that the target electrons are inert, so our results are qualitative ones. Let us first illustrate how the energy spectra depend on the polar angle of the molecular orientation. Figure 2 shows the differential cross section (DCS) for the laser-assisted potential scattering of electrons on CO molecules, as a function of the final electron energy E_f . The scattering occurs in a laser field having a wavelength of 1500 nm and an intensity of 7×10^{13} W/cm². The energy of the incident electrons is $E_i = 5$ eV, while the scattering angle is $\theta_f = 0^\circ$. The polar angle of the molecular orientation θ_m is given in each panel of Fig. 2. The energy spectra calculated with $\theta_m = 60^\circ$ and 90° show a plateau-like oscillatory structure, where the higher plateau appears in the low-energy part of the spectrum and corresponds to the single scattering, while the lower plateau appears in the

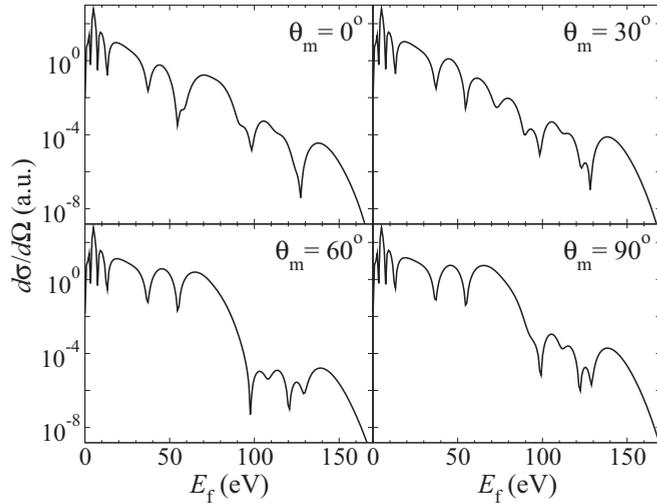


FIG. 2. The DCS for the laser-assisted potential scattering of electrons on CO molecules, as a function of the final electron energy E_f . Both the single and the double scattering are included. The wavelength and the intensity of the laser field are 1500 nm and 7×10^{13} W/cm², respectively. The incident electron energy is $E_i = 5$ eV and the scattering angle is $\theta_f = 0^\circ$. The polar angle of the molecular orientation θ_m is given in each panel.

high-energy part of the spectrum and is a consequence of the double scattering. Both plateaus end with an abrupt cutoff. As one can see, the double-scattered electrons may have higher energies in the final state than those that scattered on target only once. This plateaulike oscillatory structure is a general feature of the laser-assisted electron-atom scattering (see, for example, Refs. [13,15–17]). On the other hand, the energy spectra calculated with $\theta_m = 0^\circ$ and 30° contain a sequence of declining maxima instead of plateaus. There is still an abrupt cutoff of the energy spectrum when the maximum possible value of the final electron energy in the double-scattering process is reached, but one cannot observe the cutoff for the single-scattering process. Therefore, we cannot distinguish between the single-scattering and double-scattering parts of the spectrum. This structure of the energy spectra for $\theta_m = 0^\circ$ and 30° can be explained by the two-center interference effects that occur in the electron-molecule scattering process.

Our T -matrix element for the electron-molecule scattering is defined by Eqs. (8) and (15) and it consists of two terms. The first term describes the single scattering and may be written as

$$T_{fi}^{(1)}(n) \equiv T^{\text{tot1}} = T^A + T^B, \quad (28)$$

where T^A and T^B are the partial T -matrix contributions that correspond to the electron scattering on the atomic centers A and B , respectively. The second term of the T -matrix element describes the double scattering and may be written as

$$T_{fi}^{(2)}(n) \equiv T^{\text{tot2}} = T^{A-A} + T^{B-B} + T^{A-B} + T^{B-A}, \quad (29)$$

where T^{A-A} (T^{B-B}) corresponds to the double scattering on the center A (B), while T^{A-B} (T^{B-A}) corresponds to the scattering on the center A (B) followed by the scattering on the center B (A). Let us first analyze the two-center interference in the single-scattering process. An example is shown in Fig. 3,

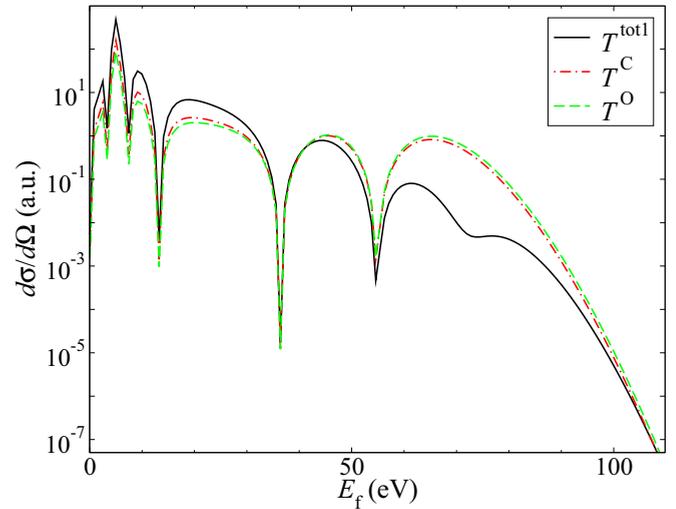


FIG. 3. The DCS for the laser-assisted potential scattering of electrons on CO molecules, as a function of the final electron energy E_f . Only the single scattering is included. All parameters are the same as in the top right panel of Fig. 2, for which $\theta_m = 30^\circ$. The partial contributions to the single-scattering process are presented along with the total contribution, as denoted in the legend.

where the DCS for the laser-assisted potential scattering of electrons on CO molecules is presented as a function of the final electron energy E_f . All parameters are the same as in the top right panel of Fig. 2. The total contribution is compared with the partial contributions to the single-scattering process. As one can see from Fig. 3, the constructive interference occurs for $0 \text{ eV} < E_f < 35 \text{ eV}$, while the rest of the energy spectrum ($E_f > 35 \text{ eV}$) is characterized by the destructive interference. Due to these two-center interference effects, the total DCS is increased for $E_f < 35 \text{ eV}$ and decreased for $E_f > 35 \text{ eV}$. The energy spectrum of the electron-molecule single-scattering process is featured by a sequence of declining maxima instead of a relatively flat, plateaulike, oscillatory structure.

An analysis of the two-center interference in the double-scattering process is illustrated in Fig. 4, where the DCS for the laser-assisted potential scattering of electrons on CO molecules is presented as a function of the final electron energy E_f and all parameters are the same as in the top right panel of Fig. 2. The total contribution is compared with the partial contributions to the double-scattering process. The results presented in Fig. 4 clearly point to the destructive interference for $53 \text{ eV} < E_f < 88 \text{ eV}$, while the rest of the energy spectrum features constructive interference. The relevant part of the double-scattering spectrum is the one that is not masked by the single-scattering contribution when both single and double scattering are included. In the considered case, it is the part where $E_f > 90 \text{ eV}$. Therefore, we can conclude that the relevant part of the double-scattering spectrum is characterized by constructive interference. The final result is a decreased difference between the single-scattering contribution in the middle-energy region ($35 \text{ eV} < E_f < 90$) and the double-scattering contribution in the high-energy region ($E_f > 90 \text{ eV}$). This is the reason why a characteristic plateaulike oscillatory structure is replaced by a sequence of declining maxima in the energy spectrum.

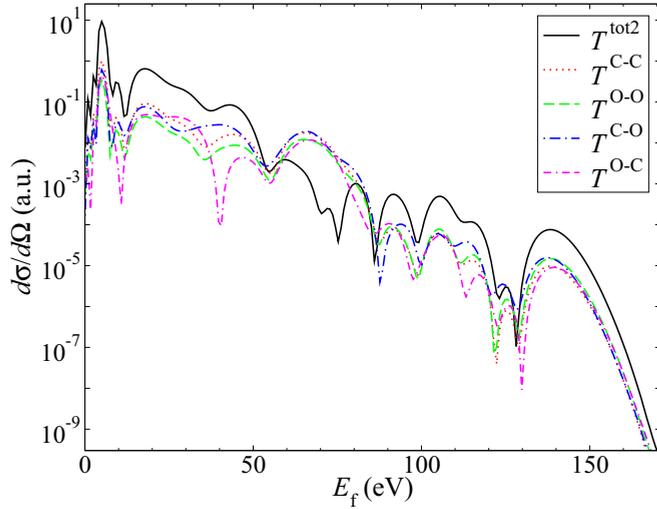


FIG. 4. Same as in Fig. 3 but with only the double scattering included. Partial contributions and the total contribution to the double-scattering process are presented, as denoted in the legend.

We now turn our attention to the two-center destructive interference minima in the energy spectra of the laser-assisted electron-molecule scattering. In the case of homonuclear diatomic molecules, these minima are determined by Eqs. (23) and (27) for single and double scattering, respectively. If $\theta_m = 90^\circ$, Eqs. (23) and (27) have the same form and the destructive interference minima for single and double scattering are given by

$$k_{f,n} = \frac{(2n+1)\pi}{R_0 \cos(\theta_f - 90^\circ)} \quad (n = 0, 1, 2, \dots). \quad (30)$$

Therefore, if $\theta_m = 90^\circ$, the destructive interference minima for single and double scattering occur at the energy values

$$E_{f,n} = \frac{k_{f,n}^2}{2} = \frac{(2n+1)^2 \pi^2}{2R_0^2 \cos^2(\theta_f - 90^\circ)} \quad (n = 0, 1, 2, \dots). \quad (31)$$

We will display these interference minima for N_2 and Ar_2 molecules. The DCS for the laser-assisted potential scattering of electrons on N_2 molecules is presented as a function of the final electron energy E_f in Fig. 5. The scattering process is assisted by a laser field having a wavelength of 1500 nm and an intensity of 10^{14} W/cm². The energy of the incident electrons is $E_i = 5$ eV, while the electron scattering angle is $\theta_f = 30^\circ$. The polar angle of the molecular orientation is $\theta_m = 90^\circ$. According to Eq. (31), the destructive interference minimum for $n = 0$ should appear at $E_{f,0} = 124.3$ eV ($R_0 = 2.08$ a.u. for N_2 , with $\theta_f = 30^\circ$) and one can see that the lowest minimum in Fig. 5 appears exactly at this value of the final electron energy.

A better illustration of the destructive interference minima is given by Fig. 6, where the logarithm of the DCS for the laser-assisted potential scattering of electrons on N_2 molecules is presented in false colors, as a function of the final electron energy E_f and scattering angle θ_f . The other parameters are the same as in Fig. 5. The two-center destructive interference minima corresponding to various values of the scattering angle

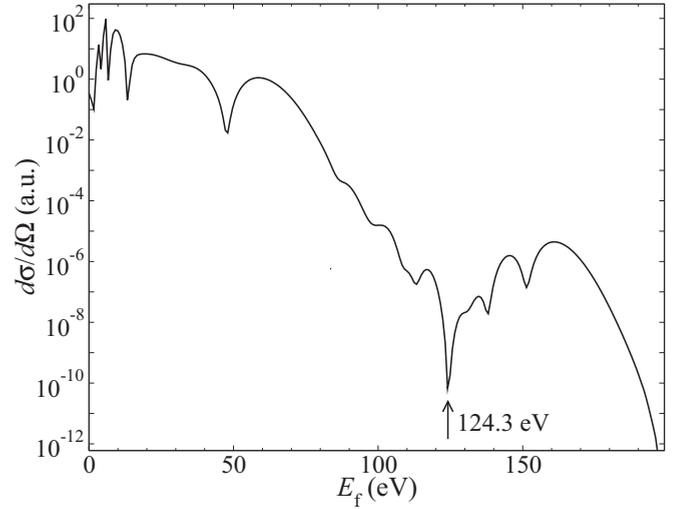


FIG. 5. The DCS for the laser-assisted potential scattering of electrons on N_2 molecules, as a function of the final electron energy E_f . Both the single and the double scattering are included. The wavelength and the intensity of the laser field are 1500 nm and 10^{14} W/cm², respectively. The incident electron energy is $E_i = 5$ eV and the scattering angle is $\theta_f = 30^\circ$. The polar angle of the molecular orientation is $\theta_m = 90^\circ$.

θ_f form a symmetric U-shaped structure in the angle-resolved energy spectrum, as one can see from Fig. 6. The positions of all these interference minima in the angle-resolved energy spectrum are accurately predicted by Eq. (31) and they all correspond to $n = 0$. Figures 5 and 6 show that there is only one destructive interference minimum in the energy spectrum of the laser-assisted electron- N_2 -molecule scattering for a specific value of the scattering angle θ_f . This is due to a relatively small equilibrium internuclear distance R_0 in the N_2 molecule ($R_0 = 2.08$ a.u. for N_2).

If we consider the scattering of electrons on molecular targets having a larger internuclear distance, we may expect more two-center destructive interference minima in the energy spectrum. Such an example is illustrated in Fig. 7, where the

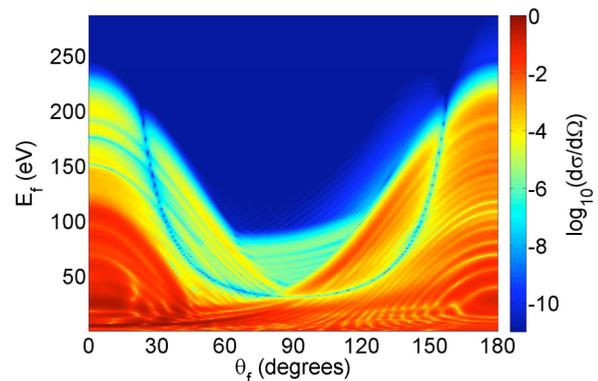


FIG. 6. Logarithm of the DCS for the laser-assisted potential scattering of electrons on N_2 molecules, presented in false colors, as a function of the final electron energy E_f and scattering angle θ_f . The other parameters are the same as in Fig. 5. Both the single and the double scattering are included.

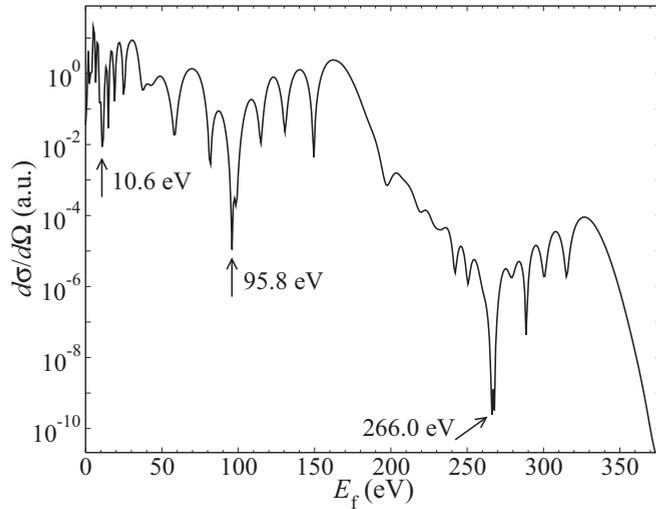


FIG. 7. The DCS for the laser-assisted potential scattering of electrons on Ar_2 molecules, as a function of the final electron energy E_f . Both the single and the double scattering are included. The wavelength and the intensity of the laser field are 1500 nm and $2 \times 10^{14} \text{ W/cm}^2$, respectively. The incident electron energy is $E_i = 5 \text{ eV}$ and the scattering angle is $\theta_f = 30^\circ$. The polar angle of the molecular orientation is $\theta_m = 90^\circ$.

DCS for the laser-assisted potential scattering of electrons on Ar_2 molecules is presented as a function of the final electron energy E_f . The scattering occurs in a laser field having a wavelength of 1500 nm and an intensity of $2 \times 10^{14} \text{ W/cm}^2$. The incident electron energy is $E_i = 5 \text{ eV}$, the scattering angle is $\theta_f = 30^\circ$, and the polar angle of the molecular orientation is $\theta_m = 90^\circ$. As $\theta_f = 30^\circ$ and the equilibrium internuclear distance in the Ar_2 molecule is $R_0 = 7.11 \text{ a.u.}$, Eq. (31) predicts the destructive interference minima at $E_{f,0} = 10.6 \text{ eV}$, $E_{f,1} = 95.8 \text{ eV}$, and $E_{f,2} = 266.0 \text{ eV}$ for $n = 0, 1$, and 2 , respectively. Figure 7 shows that three minima in the energy spectrum appear exactly at these values of the final electron energy. There are many minima in the energy spectrum presented in Fig. 7, so we cannot distinguish between the two-center destructive interference minima and other types of minima without using Eq. (31). Thus, we need Eq. (31) to identify the three minima produced by the two-center destructive interference. However, these three minima are easily distinguishable from other types of minima in the angle-resolved energy spectrum.

Such a spectrum is displayed in Fig. 8, where the logarithm of the DCS for the laser-assisted potential scattering of electrons on Ar_2 molecules is presented in false colors, as a function of the final electron energy E_f and scattering angle θ_f . The other parameters are the same as in Fig. 7. One can clearly see three symmetric U-shaped structures in the angle-resolved energy spectrum that is presented in Fig. 8. These U-shaped structures are formed by the two-center destructive interference minima that correspond to various values of the scattering angle θ_f . Positions of all these interference minima in the angle-resolved energy spectrum are accurately predicted by Eq. (31). The interference minima that form the lowest, the middle, and the highest U-shaped structure in Fig. 8 correspond to $n = 0, 1$, and 2 in Eq. (31), respectively. The analysis

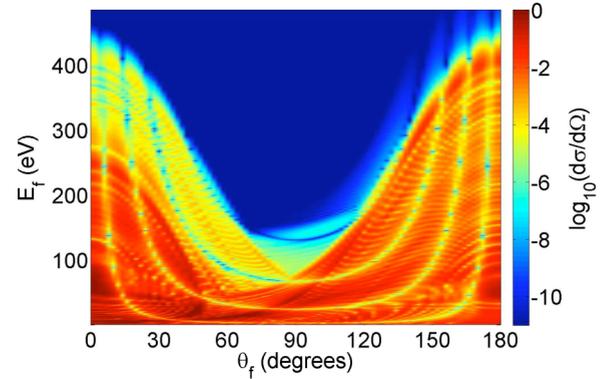


FIG. 8. Logarithm of the DCS for the laser-assisted potential scattering of electrons on Ar_2 molecules, presented in false colors, as a function of the final electron energy E_f and scattering angle θ_f . The other parameters are the same as in Fig. 7. Both the single and the double scattering are included.

presented above leads us to the conclusion that positions of the two-center destructive interference minima in the energy spectra of the laser-assisted electron-molecule scattering may be calculated by simple analytical formulas in the case of homonuclear diatomic molecules.

V. CONCLUSION

It is well known that the energy spectra of various atomic and molecular processes in the laser field show a plateau-like oscillatory structure. The plateaus in the energy spectra are formed by a series of maxima and minima that are a consequence of the interference of the partial contributions to the process. These partial contributions correspond to different electron trajectories in the laser field, i.e., every possible electron trajectory in the laser field contributes to the total yield for the process. As the molecules are multicenter systems, the energy spectra of the molecular processes in the laser field are characterized by additional interference effects. These multicenter interference effects are responsible for an increase or a decrease of the yield of the total process in a specific part of the energy spectrum. They also produce additional minima in the energy spectrum.

We have analyzed the laser-assisted potential scattering of electrons on diatomic molecules. Our analysis has shown that, for certain molecular orientations, the familiar plateaus in the energy spectrum of scattered electrons are replaced by a sequence of gradually declining maxima. Such a behavior of the energy spectra can be explained by the two-center interference effects that occur in the electron-molecule scattering process.

We have also shown that, in the case of homonuclear diatomic molecules, the positions of the two-center destructive interference minima in the energy spectra of the laser-assisted electron-molecule scattering may be determined by simple analytical formulas. This has been illustrated for N_2 and Ar_2 molecules. The number of two-center destructive interference minima that appear in the energy spectrum depends on the internuclear distance in the molecular target. The larger the internuclear distance, the larger the number of destructive interference minima. Therefore, the energy spectrum of the

laser-assisted electron–Ar₂-molecule scattering shows a larger number of destructive interference minima than that of the laser-assisted electron–N₂-molecule scattering. If the molecular axis is perpendicular to the incident electron momentum and to the unit polarization vector of the laser field, i.e., if $\theta_m = 90^\circ$, the two-center destructive interference minima for the single scattering appear at the same values of final electron energy as those for the double scattering. In this case, the

two-center destructive interference minima form symmetric U-shaped structures in angle-resolved energy spectra.

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