A four-component Dirac theory of ionization of a hydrogen molecular ion in a super-intense laser field

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Abstract

In this communication, a four-component Dirac theory of ionization of a hydrogen molecular ion, H$_2^+$, in a super-intense laser field is presented. Analytic expressions for the spin-specific as well as the total ionization currents emitted from the ground state of the ion are derived. The results are given for arbitrary intensity, frequency, wavenumber and polarization of the field, and for the up or down spin of the bound and ionized states of the electron. They also apply for the case of inner-shell ionization of analogous heavier diatomic molecular ions. The presence of molecular two-slit interference effect, first found in the non-relativistic case, the spin-flip ionization current, and an asymmetry of the up- and down-spin currents similar to that predicted in the atomic case, is found to hold for the present relativistic molecular ionic case as well. The possibility of controlling the spin of the dominant ionization current in any direction by simply selecting the handedness of a circularly polarized incident laser field is pointed out. Finally, we note that the present results obtained within the strong field ‘KFR’ ansatz open up the way for an analogous fully relativistic four-component treatment for ionization of polyatomic molecules and clusters in super-intense laser fields.

1. Introduction

In view of the rapid progress in ultra-short laser pulse techniques and high-frequency FEL technology, super-intense laser fields reaching intensities $\geq 10^{22}$ W cm$^{-2}$, and FEL radiations of intensities $\geq 10^{16}$ W cm$^{-2}$ are now available or expected to be available in laboratories in the near future. The purpose of this communication is to present for the first time a four-component Dirac theory of ionization of the simplest of molecules, H$_2^+$, and of the analogous but heavier K-shell molecular ions by super-intense laser fields of arbitrary frequency, wavenumber and polarization. The present relativistic approach within the strong-field ‘KFR’ ansatz [1, 2] is a generalization of the method developed earlier for the atomic case [2] to the case of a molecular ion.

A non-perturbative relativistic analysis of intense-field ionization dynamics becomes necessary (a) if the laser is super-intense, i.e. so high that the ponderomotive energy $U_p = \frac{e^2 F^2}{2 m_0 c^2}$ becomes comparable to or greater than the rest-mass energy $m_0 c^2$ of the electron, $U_p \geq m_0 c^2$; (b) if the spin degrees of freedom, the magnetic field component and/or the retardation effect of the field become significant; or (c) if the initial bound electron is in a deep-lying shell of the target molecule or its ions, where the electron motion is already relativistic without the laser field. We may recall that the velocity of a K-shell electron in an atom of nuclear charge $Z$ is given by $v/c = Z\alpha$, so that for $Z \approx 70$, the corresponding velocity is more than 50% of the velocity of light. It should be noted further that although initially a bound electron may be in the upper valence shell—where its motion can be non-relativistic ($v/c \ll 1$)—a super-intense laser pulse could, nevertheless, strip the target molecule of the outer-shell electrons before the peak of the pulse arrives. Thus effectively the pulse at its highest intensities might in fact interact with the relativistically moving electrons of the inner shells of the stripped ions and ionize them further. Also, an initially non-relativistically moving outer-shell electron on virtual ionization at low velocities might be accelerated to relativistic velocities by the ultra-intense laser.
pulse. Furthermore, intense high-frequency free electron laser (FEL) radiation can interact directly and strongly with the relativistically moving bound electrons in the deep-lying shells of atoms and molecules. With these considerations in mind, in this work we demonstrate how a fully relativistic (four-component Dirac) theory of ionization of K-shell molecular ions could be achieved within the intense-field KFR ansatz [1, 2]. It is well known that the latter ansatz has been very fruitful in the non-relativistic treatment of ionization (as well as other dynamical processes such as high harmonic generation) from atoms and molecules in intense low-frequency laser fields in the past (for a review, see, e.g. [6]).

2. Theoretical formulation

The Dirac equation of a diatomic molecular ion interacting with an intense electromagnetic field can be written as

\[ \frac{\partial \Psi(t)}{\partial t} = \left[ c\alpha \cdot \left( p_{op} - \frac{e_0}{c} A(\omega t - \kappa \cdot r) \right) - \frac{Z_a e_0^2}{r_a} - \frac{Z_b e_0^2}{r_b} + \beta m_0 c^2 \right] \Psi(t). \]  

(1)

where \( m_0 \) and \( e_0 \) are the rest mass and charge of the electron, \( \alpha \) and \( \beta \) are the standard Dirac 4 x 4 matrices, and \( V_f(t, r) = -e_0 \alpha \cdot A(u) \), with \( u = (\omega t - \kappa \cdot r) \), is the electron–laser interaction Hamiltonian and \( A(u) \) is the vector potential of the external radiation field:

\[ A(\omega t - \kappa \cdot r) = A_0 e_1 \cos(\xi/2) \cos(\omega t - \kappa \cdot r) \]

- \( e_2 \sin(\xi/2) \sin(\omega t - \kappa \cdot r) \)  

(2)

We consider the general case of a laser field of arbitrary elliptic polarization (ellipticity parameter \( \xi [0, \pi/2] \); \( \xi \) stand for the left and right helicity) with the semi-major and the semi-minor unit polarization vectors \( e_1 \) and \( e_2 \), respectively. It should be noted that the Coulomb fields of the ‘heavy’ nuclei a and b are the locations of the two nuclei a and b, respectively. Clearly, for the homonuclear diatomic case (C.M. of the nuclei as coordinate center), \( R_a = -R_b = R/2 \) where R is the nuclear separation, and \( Z_a = Z_b = Z \) is the nuclear charge.

We introduce the initial state partition of the total Dirac Hamiltonian

\[ H_D(t) = H_{mol} + V_f(u) \]

(3)

where \( V_f(u) = -e_0 \alpha \cdot A(u) \), and

\[ H_{mol} = \left[ c\alpha \cdot p_{op} - \frac{Z_a e_0^2}{r_a} - \frac{Z_b e_0^2}{r_b} + \frac{Z_a Z_b e_0^2}{R} + \beta m_0 c^2 \right] \]  

(4)

is the molecular Dirac Hamiltonian, with stationary eigenfunctions satisfying the Dirac equation:

\[ (E - H_{mol}) \psi_r(r) = 0 \]  

(5)

with positive and/or negative energy eigenvalues \( E_r \). We choose the final state partition of the total Dirac Hamiltonian \( H_D(t) \) (given by the right-hand side of equation (1)) as

\[ H_D(t) = H_{vol}(t) + V_f(u) \]

where

\[ H_{vol}(t) = \left( c\alpha \cdot \left( p_{op} - \frac{e_0}{c} A(u) \right) + \beta m_0 c^2 \right) \]  

(6)

is the Dirac–Volkov Hamiltonian of an electron in the plane wave field, equation (2), and

\[ V_f = V_{mol}(r; R) = -\frac{Ze_0^2}{r_a} - \frac{Ze_0^2}{r_b} + \frac{Z_a Z_b e_0^2}{R}. \]

(7)

For ease of working with Dirac equations it is useful to reduce the number of four natural constants appearing in them to only two by introducing the reduced constants: \( m = \frac{m_0}{\sqrt{\epsilon_0} \gamma} \) and \( \epsilon = \frac{\gamma}{\gamma^2} \) (which can be therefore restored easily at the end, if desired), and the following Feynman notations for 4-vector, 4-scalar product and the 4-gamma matrices:

\[ \begin{align*}
\phi &= \phi^\dagger \gamma_0 \\
\bar{\phi} &= \phi \gamma_0 \\
d^4x &= d\xi_0 dx \\
\end{align*} \]

In this notation, for example, equation (1) takes the form

\[ (i\gamma \cdot p - m_0)\bar{\psi}(x; R) = 0 \]

(9)

The total Dirac wavefunction can be expanded systematically, as in the non-relativistic ‘intense-field many-body S-matrix theory’ (or IMST, see the review [6]), in terms of the Dirac–Volkov–Feynman Green’s function \( G_F(x, x’) \) that satisfies

\[ (i\gamma \cdot p - m)G_F(x, x’) = \delta^4(x - x’) \]

(10)

A complete set of solutions [7] of the Dirac–Volkov equation (6) can be conveniently written as

\[ \Phi^{(i)}(x) = \int_{-\infty}^{m} \frac{m}{\sqrt{E - \frac{e \alpha \cdot A(u)}{2p \cdot \kappa}}} \left( 1 + \frac{e \alpha \cdot A(u)}{2p \cdot \kappa} \right) \]  

(11)

where for a general pulse of a transverse external electromagnetic wave, \( A(u) \), we get

\[ f_p(x) = \int_{-\infty}^{+\infty} \frac{m}{\sqrt{E - \frac{e \alpha \cdot A(u)}{2p \cdot \kappa}}} \]  

(12)

For a vector potential of a constant envelope it reduces to (in a.u.)

\[ f_p(x) = -a_p \sin(x + \chi_p) + b_p \sin(2u) + \xi_p \]  

(13)

(14)
where $E \equiv \sqrt{(p^2 + m^2)}$. The up and down positive energy 4-spinors $w_{j}^{(s)}$ are given by

$$w_{j}^{(1a)} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad (15a)$$

and

$$w_{j}^{(2a)} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}. \quad (15b)$$

Similarly, the up and down negative energy 4-spinors are

$$w_{j}^{(3a)} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad (16a)$$

and

$$w_{j}^{(4a)} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \quad (16b)$$

Thus, the Dirac–Volkov Green’s function satisfying the Feynman–Stückelberg boundary condition (cf [8]) can be defined by

$$G_F(x, x') = -i \left( \frac{\hbar}{E} \right) \sum_p \left( \sum_{i=1,2} \theta(t - t') \Phi_p^{(i)}(x) \Phi_p^{(i)}(x') \right)$$

$$+ \sum_{j=1,2,4} \theta(t - t') \Phi_p^{(j)}(x) \Phi_p^{(j)}(x') \right), \quad (17)$$

where $\sum_p = \frac{1}{(2\pi)^3} \int d^3 p$. For an explicit momentum representation of $G_F(x, x')$, which can be used conveniently for intense periodic electromagnetic fields, we refer to [5] or equation (54) of [6].

Using $G_F(x, x')$ one may systematically solve equation (9) by iteration, to obtain the total Dirac state evolving from a specified initial state $\psi_i^{(s)}(x)$:

$$\Psi_j(x) = \psi_j^{(s)}(x) + \int_{x_0}^{x_1} d^3 x' G_F(x, x')(e \mathcal{A}(x')) \psi_j^{(s)}(x')$$

$$+ \int_{x_0}^{x_1} d^3 x' \int_{x_0}^{x_1} d^3 x'' G_F(x, x'')(\gamma_0 V_f(x''))$$

$$\times G_F(x'', x')(e \mathcal{A}(x'')) \psi_j^{(s)}(x'') + \cdots, \quad (18)$$

where $V_f(x)$ is the rest potential in the final state. This constitutes the Dirac wavefunction within the ‘relativistic intense-field many-body S-matrix theory’ (or RIMST) subjected to the Feynman–Stückelberg backward-time positron interpretation of the negative energy ‘Dirac sea’. It should be noted, therefore, that the present approach can be used for obtaining the probability of not only ionization, as we consider in this work, but also of such processes as pair creation in super-intense laser fields (cf [8]).

3. Ground state $H_2^+$ molecular ion in a Dirac basis

We shall represent the ground state four-component wavefunction $\psi_i^{(s)}(x)$, of hydrogenic molecular ions, in the spin state, $s = (u, d)$, by a linear combination of relativistic atomic basis orbitals of $\sigma$ symmetry. To this end we define a four-component ‘Dirac basis’ (with $\sigma$ symmetry) of the form

$$\phi_j^{(s)}(r) = R_j(r) \psi_{j,\pm}(\hat{r}) u_j^{(s)}; \quad j = 1, 2, 3, \ldots, \quad (19)$$

$$R_j(r) = N_j r^{v_j - 1} e^{-\lambda_j r}, \quad (20)$$

where $\psi_{j,\pm}(\hat{r}) = \gamma \cdot n_j,\pm(\hat{r})$ and the 4-vector $n_j,\pm(\hat{r}) = (n_0, \pm n_j(\hat{r}))$, with $n_0 = 1$, $n_j(\hat{r}) = i \beta_j \hat{r}$ and $\beta_j = \frac{\lambda_j}{\nu_j}$, where $\nu_j$ and $\lambda_j$ are in general non-integer real parameters and $N_j = (2\lambda_j)^{
u_j + 1} \left( \frac{1 + \nu_j}{1 + \nu_j/2} \right)^{1/2}$ is a normalization constant. Note that the well-known hydrogenic Dirac s-state wavefunctions [9] in the present notation (from [10], p. 418) can be reproduced by choosing a single Dirac basis state with $v_0 = \sqrt{1 - (Z\alpha)^2}$ and $\lambda_1 = m Z \alpha$, where $\alpha$ is the fine structure constant and $Z$ is the nuclear charge. The Fourier transforms of the Dirac basis functions introduced above are evaluated analytically and we get

$$\phi_j^{(s)}(q) = \int d^3 r e^{-iq\cdot r} \phi_j^{(s)}(r)$$

$$= N_j \epsilon_j(q)[1 \pm g_j(q)(\gamma \cdot \hat{q})] u_j^{(s)}, \quad (21)$$

where

$$\epsilon_j(q) = \int e^{-\hat{q}\cdot \tau} r^{v_j - 1} e^{-\lambda_j r} d^3 r$$

$$= \frac{4\pi \Gamma(1 + v_j)}{q(q^2 + \lambda_j^2)^{1/2}} s_j(q), \quad (22)$$

and

$$s_j(q) = \sin((v_j + 1) \arctan(q/\lambda_j)) \quad (23)$$

The corresponding negative energy basis functions can be obtained from the F.T. (momentum representation) of the above positive energy basis functions by letting $q \rightarrow -q$, and replacing the positive energy up and down spinors $u_j^{(s)}$, $s = (1, 2)$, by the negative energy up and down spinors $u_j^{(s)}$, $s = (3, 4)$, defined above. Finally, we write the Dirac $H_2^+$ ground state wavefunction as

$$\psi_i^{(s)}(r; R) = \sum_j a_j [R_j(r_a) \psi_{j,\pm}(\hat{r}_a) u_j^{(s)}$$

$$+ R_j(r_b) \psi_{j,\pm}(\hat{r}_b) u_j^{(s)}] \quad (25)$$

where $a_j$ are numerical constants, and $u_j^{(s)}$ are the positive energy spinors defined above.
4. Ionization transition amplitude: up- and down-spin currents

Projecting the final Volkov state of 4-momentum $p$, equation (11), on the total wavefunction $\Psi_i(x)$, and retaining the leading significant term, we get the individual spin selected ionization amplitudes ($s = u$ or $d$ to $s' = u$ or $d$):

$$A_{\text{ion}}(s \rightarrow s') = -i \int d^4x \, \Phi^{(r)}(x) e^{i A(x) \psi_i^{(s)}(x)}. \quad (26)$$

Using the Fourier transform of the ground state wavefunction, carrying out the $d^4x$ integration, and performing the somewhat lengthy Dirac $\gamma$-algebra, we arrive at the following explicit analytic result (in a.u. $\epsilon_0 = m_0 = \hbar = ac = 1$):

$$A_{\text{ion}}(s \rightarrow s') = 2\pi i \sum_n \delta(p_0 - p_0 - (\zeta_p - n)\kappa_0) T^{(n)}(s', s) \quad (27)$$

with

$$T^{(n)}(s', s) = \frac{A_0}{2c} N_{p_0}(t^{(s)}_n(s', s) e^{i\eta R_n} + t^{(s)}_n(s', s) e^{i\eta R_n}) \quad (28)$$

$$t^{(s)}_n(s', s) = \sum_j a_j N_{p_0}(0) M^{(g)}_j(s', s; \pm g_j). \quad (29)$$

Given the matrix elements $M^{(s)}_j(s', s; \pm g_j)$, the spin-specific rates of ionization become

$$dW_{\text{ion}^{s' \rightarrow s}} = \sum_{n \geq n_0} \left( \frac{A_0}{2c} N_{p_0} \right)^2 |T^{(n)}(s', s)|^2 \frac{2 c_0 |p_0|}{(2\pi)^2}$$

$$= \sum_{n \geq n_0} \left( \frac{A_0}{2c} N_{p_0} \right)^2 \left| t^{(s)}_n(s', s) e^{i\eta R_n} + t^{(s)}_n(s', s) e^{i\eta R_n} \right|^2 \frac{2 c_0 |p_0|}{(2\pi)^2} \quad (30)$$

The number of absorbed photons (denoted by $n$ above, where $n_0$ is the threshold number) is determined by the 4-momentum conservation relation, obtained from the delta function that appears naturally in equation (27) from the spacetime integration: $n \omega = \epsilon_0 + \epsilon_{km} + \zeta_p \omega$, where $\epsilon_0 = c (c - \sqrt{c^2 - p^2})$ is the binding energy (ionization potential) and $\epsilon_{km} = c (\sqrt{c^2 + p^2} - c)$ is the kinetic energy. On completing the Dirac algebra, the reduced $M^{(s)}_j(s', s; g_j)$-matrix elements are found to be given by the following simple algebraic expressions:

$$M^{(n)}_j(u \rightarrow u; g_j) = B^{(n)}_u (m_1 + m_2 g_j(q) (\hat{p} \cdot \hat{q} - i (\hat{p} \times \hat{q})))$$

$$+ B^{(n)}_u (m_2 \hat{p} + m_1 g_j(q) \hat{q})$$

$$- i B^{(n)}_u (m_2 \hat{p} - m_1 g_j(q) \hat{q}) \chi, \quad (31)$$

$$M^{(n)}_j(u \rightarrow d; g_j) = m_2 g_j(q) B^{(n)}_u (i (\hat{p} \times \hat{q}) + (\hat{p} \times \hat{q})), \quad (32)$$

$$M^{(n)}_j(d \rightarrow u; g_j) = m_2 g_j(q) B^{(n)}_u (i (\hat{p} \times \hat{q}) - (\hat{p} \times \hat{q})), \quad (33)$$

are generalized Bessel functions of three arguments. The other parameters are the ‘field-dressed’ electron momentum $q = q_0 + (\zeta_p - n)\kappa_0$, $\zeta_p = \frac{1}{4c^2 - p^2}$, $e(\xi) = \left[ e_1 \cos \left( \frac{\xi}{2} \right) + ie_2 \sin \left( \frac{\xi}{2} \right) \right]$, with $\xi = [0, \pm \pi/2]$, $p_0 = \sqrt{c^2 + p^2} = (n - \zeta_p)\kappa_0 + \sqrt{c^2 - p^2}$, $m_1 = \sqrt{(p_0 + c)/(2c)}$, $m_2 = \sqrt{(p_0 - c)/(2c)}$ and $N_{p_0} = \sqrt{\frac{c_0}{p_0}}$.

Finally, the spin unresolved total ionization rate from an unpolarized target atom is obtained by simply adding the four spin-specific rates given above and dividing by 2 (for the average with respect to the two degenerate initial spin states):

$$\frac{d\Gamma^{(s)}}{d\Omega} = \frac{1}{2} \sum_{\langle s' = u | s \rangle} \sum_{n \geq n_0} \left( \frac{A_0}{2c} N_{p_0} \right)^2 \left| t^{(s)}_n(s', s) e^{i\eta R_n} \right|^2 \frac{2 c_0 |p_0|}{(2\pi)^2} \quad (39)$$

We may point out that equations (28), (30) and (39) that apply directly for the ‘$\sigma_u$’ case, can be used to obtain also the probability of ionization from an analogous ‘$\sigma_g$’ case, if one simply replaces the sum (‘+’) of the two interfering nuclear terms in these formulas with their difference (‘-’).

4.1. Ionization probability and molecular two-slit interference

It is interesting to see from equations (28), (30) and (39) that the ionization amplitude and the probabilities do not exactly factorize into two factors, one of which depends on the nuclear geometry and the other on the electronic degrees of freedom. The geometrical factor leads to an interference effect arising from the superposition of the partial electronic waves that emerge from the two nuclear centers with a phase difference $q \cdot (R_b - R_a) = q \cdot R$. This leads to the now well-known molecular two-slit interference (and its dependence on the symmetry of the electronic wavefunction of the active electron) first discussed in the non-relativistic case [3]. Thus for example, for the ionization probability from the ‘$\sigma_g$’ molecular orbital of $H_2^+$, the two-slit interference factor becomes: $|1 + \lambda e^{i\theta} R^2|$, with $\lambda \equiv \sum_{\langle s' = u | s \rangle} \sum_{n \geq n_0} \left| t^{(s)}_n(s', s) e^{i\eta R_n} \right|^2$, which for $q \cdot R = 2n\pi, n = 0, 1, 2, \ldots$, gives rise to a constructive interference and an enhancement of the ionization probability by a maximum factor of $|1 + \lambda|^2$, while for $q \cdot R = (2n + 1)\pi, n = 0, 1, 2, \ldots$, a destructive interference occurs.
yields minimum (at most $|1 - \lambda|^2$) in the energy–momentum distributions of the ionized electron. We note that the two-slit interference effect is generic in nature and can show its influence in all channels in which the active electron of the molecule determines the channel probability, not only in ionization but also e.g. in laser stimulated molecular electron diffraction, laser induced emission of (low or high) harmonic radiation, etc. Furthermore, it can survive even in the signals that are obtained in orientation averaged measurements. In this case the interference probability factor reduces to

$$\frac{1}{4\pi} \int d\Omega_R |1 + \lambda e^{i q R}|^2 = \left( 1 + |\lambda|^2 + 2N(\lambda) \frac{\sin q R}{q R} \right), \quad (40)$$

which indicates an interference modulation with the variation of the electron momentum $q$ (or $R$), albeit decreasing in the modulation-depth with increasing momentum and/or the nuclear separation $R$.

4.2. Linear and circular polarization, photon helicity and spin asymmetry

The results derived above hold for any polarization of the laser field. We note below the particular simplifications that arise in the two most common cases of linear and circular polarization.

(1) Linear polarization. In the case of a linearly polarized laser field, the explicit formulae for the ionization currents, equations (30) and (39), hold again when we simply put $\xi = 0$ in them. Thus the only change occurs in replacing the generalized Bessel function of three arguments by the generalized Bessel function of two arguments: $J_n = J_n(a_p, b_p)$, with $a_p = a_p(\xi = 0), b_p = b_p(\xi = 0)$.

(2) Circular polarization. Similarly, for the case of circular polarization of the laser field, the same expressions hold again when we simply put $\xi = \pm \pi/2$ in them. In this case, the generalized Bessel function of three arguments reduces to an ordinary Bessel function (of one argument) times a simple phase factor: $J_n = J_n(a_p) e^{i a_p \xi}$, with $a_p = a_p(\xi = \pm \pi/2)$, where $\pm$ stand for the positive and negative handedness of the circularly polarized laser field.

Closer examination of the expressions of the matrix elements $M_{j,j'}^n(s', s; \pm g_1)$ for circular polarization, as in the atomic case [2], shows that the probability of spin-flip ionization for $u \rightarrow d$ transition differs from the probability of the $d \rightarrow u$ transition. It also suggests that the up- and down-spin currents, even from a spin unpolarized (i.e. an equal mixture of up and down spin) ground state molecular ion, would show an asymmetry in any direction of the emission of the electron. This asymmetry is expected to persist also when the laser photons are of long wavelength (or the laser propagation vector $\kappa \rightarrow 0$). This implies that the dominant component of the electron spin current emitted from molecular targets by intense laser fields might be controlled by choosing the helicity of an incident circularly polarized laser field.

5. Summary

In this communication, a four-component Dirac relativistic theory of interaction of super-intense laser fields with a $H^+$ molecular ion, and its heavier K-shell analogues, is presented. To this end, a ‘Dirac basis’ of atomic orbitals is introduced and employed to construct the LCAOMO of the ground state of $H_2^+$ and similar diatomic molecular ions. Explicit analytic expressions for the probability of ionization per unit time (the rate) by an incident laser field of arbitrary intensity, wavelength and polarization are derived. The formulae obtained apply for the total ionization probability as well as for the spin-specific measurements of the ionization signal. They imply, among other things, an asymmetry of the probability of spin-flip, and of the up- and down-spin ionization currents, even from a spin unpolarized ground state molecular ion. The presence of a generic molecular two-slit interference effect, first noted in the non-relativistic case [3], is further confirmed in the present relativistic analysis. Finally the possibility of controlling the dominant spin component of the electron current emitted from the inner shell of a molecule by simply selecting the handedness of a circularly polarized incident laser field is pointed out. In conclusion, we may note that the present relativistic results open up the way for further generalizations to the more complex case of inner-shell ionization of polyatomic molecules and clusters in super-intense laser fields, by extending the non-relativistic treatment (e.g. [4]) of the latter systems to the Dirac relativistic case.

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