 Atomic ionization of hydrogen-like ions by twisted photons: angular distribution of emitted electrons

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Abstract

We investigate the angular distribution of electrons that are emitted in the ionization of hydrogen-like ions by twisted photons. Analysis is performed based on the first-order perturbation theory and the non-relativistic Schrödinger equation. Special attention is paid to the dependence of the electron emission pattern on the impact parameter \(b\) of the ion with respect to the centre of the twisted wave front. In order to explore such a dependence, detailed calculations were carried out for the photoionization of the 1s ground and 2p\textsuperscript{y} excited states of neutral hydrogen atoms. Based on these calculations, we argue that for relatively small impact parameters, the electron angular distributions may be strongly affected by altering the position of the atom within the wave front. In contrast, if the atom is placed far from the front centre, the emission pattern of the electrons is independent of the impact parameter \(b\) and resembles that observed in the photoionization by plane wave photons.

(Some figures may appear in colour only in the online journal)

1. Introduction

In the early 20th century, Einstein came up with his by now famous explanation for the photoelectric effect of UV-irradiated solid bodies [1]. Since then, the emission of electrons by light, also known as photoionization, has been studied extensively for various systems such as atoms [2–5], atomic clusters [6, 7] or molecules [8–10]. Much attention, both in experiment and theory, has been paid to the total ionization cross sections and their dependence on photon energy and electronic configurations [11–14]. Apart from the fundamental interest, these studies play an important role for the precise description of ion charge state distributions in stellar as well as laboratory plasmas [15].

Besides the total rates, the angular distributions of the photoelectrons have also been in the focus of intense research throughout the last decades [16–19]. A large number of measurements were carried out, for example, to explore the dependence of electron emission patterns on the polarization states of the incident photons [2, 3, 17]. These studies have revealed important information not only on the structure of many-electron systems but also on details of the electron–photon coupling. Owing to recent advances in photo-optics, moreover, new possibilities arise to study the photoionization of atoms and molecules, in which the incoming light will possess not only a definite polarization but also a certain projection of the orbital angular momentum (OAM) onto its propagation direction [20–22]. These special states of light, also known as twisted photons, can readily be generated in various ways, e.g., via computer-generated holograms, spiral phase plates, axicons or integrated ring resonators [21, 23–27]. The practical availability of these beams has led, moreover, to a large number of experimental investigations that focus on the role of the OAM component in light–matter interactions (for a
In order to investigate the atomic photoionization by twisted (Bessel) photons, we first need to construct the corresponding states of light in terms of the 4-vector potential $A_{\mu}(\mathbf{r},t)$. Such a potential should satisfy the wave equation

$$\left(\Delta - \alpha^2 \frac{\partial^2}{\partial t^2}\right) A_{\mu}(\mathbf{r},t) = 0,$$

which describes electromagnetic field configurations within the vacuum. Here, $\Delta$ is the Laplace operator and $\alpha$ is the electromagnetic fine-structure constant. By imposing the Coulomb gauge condition and restricting ourselves to monochromatic states of light with a well-defined energy $\omega$, we find $A_{\mu}(\mathbf{r},t) = (0, \mathbf{A}(\mathbf{r}) e^{-i\omega t}, 0)$, $\text{div} \mathbf{A}(\mathbf{r}) = 0$, (2)

where the 3-vector $\mathbf{A}(\mathbf{r})$ is a solution of the (free-space) Helmholtz equation

$$(\Delta + k^2) \mathbf{A}(\mathbf{r}) = 0.$$ (3)

In this expression, $k = \alpha \omega$ denotes the wave number of the electromagnetic field [39]. By making use of the linear momentum operator $\hat{p} = -i\nabla$, one can re-write equation (3) in the form

$$\hat{p}^2 \mathbf{A}(\mathbf{r}) = k^2 \mathbf{A}(\mathbf{r}),$$ (4)

which implies that the vector potential $\mathbf{A}(\mathbf{r})$ is an eigenfunction of the squared momentum operator.

Equations (2)–(4) describe the vector potential of an electromagnetic field that propagates in free space and include both the plane and the twisted wave solutions. For the latter case, however, some additional requirements have to be taken into account. That is, the potential $\mathbf{A}(\mathbf{r})$ for the Bessel-type twisted light is expected to be an eigenfunction of the longitudinal momentum

$$\hat{p}_z \mathbf{A}(\mathbf{r}) \equiv -i \frac{\partial}{\partial z} \mathbf{A}(\mathbf{r}) = \kappa_z \mathbf{A}(\mathbf{r})$$ (5)

and the $z$-component of the TAM operator

$$\hat{J}_z \mathbf{A}(\mathbf{r}) = m_{\mu} \mathbf{A}(\mathbf{r}),$$ (6)

where the operator $\hat{J}_z = \hat{L}_z + \hat{S}_z$ is given by the corresponding components of the OAM and SAM operators:

$$\hat{L}_z = -i \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x}\right), \quad \hat{S}_z = -i \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

(7)

From equations (4) and (5) it immediately follows, moreover, that the twisted photon is also characterized by a definite modulus of the transverse linear momentum

$$|k_{\perp}| \equiv \kappa = \sqrt{k_x^2 - k_z^2}.$$ (8)
Having characterized the twisted photon state by equations (3)–(8), we are now ready to find the explicit form of the vector potential \( \mathbf{A}(\mathbf{r}) \). As will be shown in the following two sections, this requires an analysis of the orbital and spin properties of the Bessel solutions.

2.1. Orbital structure of twisted states

As seen from the discussion above, the vector potential \( \mathbf{A}(\mathbf{r}) \) of the twisted light is an eigenfunction of the \( z \)-component and of the square of the linear momentum operator \( \hat{p} \). In order to construct such solutions, we first note that the scalar function

\[
\psi_{sk,m}(\mathbf{r}) = \frac{1}{2\pi} J_m(r_e \rho_e) e^{ik_z z}
\]

(9)

also satisfies equations (4) and (5). In this expression, we used cylindrical coordinates \( (r_e, \theta_e, z) = (\sqrt{x^2 + y^2}, \arctan(y/x), z) \) and the Bessel function \( J_m(x) \) of the first kind [40]. The function \( \psi_{sk,m}(\mathbf{r}) \) is normalized, moreover, as

\[
\int \psi_{sk,m}^*(\mathbf{r}) \psi_{sk,m}(\mathbf{r}) \, d^3r = 2\pi \delta(\chi - \chi')\delta(k_z - k'_z)\delta_{m,m'}.
\]

(10)

and can be expressed as a superposition of plane waves

\[
\psi_{sk,m}(\mathbf{r}) = \int a_{skm}(k_z) e^{ik_z z} d^2k_z = \int a_{skm}(k_z) e^{i(k_z r + k_z z)} d^2k_z.
\]

(11)

Here, each (plane wave) component is weighted by the amplitude

\[
a_{skm}(k_z) = \sqrt{\frac{2\pi}{\chi}} (-1)^m e^{im\phi_e} \delta(k_z - \chi),
\]

(12)

with \( k_z = |k_z| \) being the absolute value of the transverse momentum and \( \phi_e \) the azimuthal angle of the photon’s wave vector \( \mathbf{k} \), which, therefore, can be written as

\[
\mathbf{k} = \left( \frac{k_z \cos \phi_e}{k_z \sin \phi_e}, 1 \right).
\]

(13)

We note that for fixed values of the transversal \( \chi \) and longitudinal \( k_z \) components of the linear momentum, all wave vectors \( \mathbf{k} \) contributing to integral (11) lie on a (momentum) cone with an opening angle \( \theta_0 = \arctan(\chi/k_z) \).

The properties of the scalar function \( \psi_{sk,m}(\mathbf{r}) \) can be deduced directly from equations (11) and (12). Namely, while the delta distribution \( \delta(k_z - \chi) \) in the amplitudes (12) ensures that condition (8) is fulfilled, the factor of \( e^{ik_z z} \) in equation (11) provides for requirement (5). Moreover, in the momentum space, where \( \hat{L}_z = -i \frac{\partial}{\partial \chi} \), the amplitude \( a_{skm}(k_z) \) is an eigenfunction of the OAM operator

\[
\hat{L}_z a_{skm}(k_z) = m_l a_{skm}(k_z).
\]

(14)

By performing the Fourier transformation on both sides of equation (14) in the two-dimensional \( k_z \)-space and by multiplying with \( e^{ik_z z} \), we find that a similar relation holds for the function \( \psi_{sk,m}(\mathbf{r}) \) in the coordinate space

\[
\hat{L}_z \psi_{sk,m}(\mathbf{r}) = m_l \psi_{sk,m}(\mathbf{r}).
\]

(15)

2.2. Spin structure of twisted states

Before the requirements (4), (5) and (8) which define the orbital structure of the twisted Bessel light, the vector potential \( \mathbf{A}(\mathbf{r}) \) has to be an eigenfunction of the (\( z \)-projection of the) TAM operator \( \hat{J}_z = \hat{L}_z + \hat{S}_z \) (cf equation (6)), Therefore, to construct the \( \mathbf{A}(\mathbf{r}) \) we have to specify also its spin properties. Along this line, let us first remind how one describes the spin-polarization properties of the standard plane wave solutions of the Helmholtz equation (3). Within the Coulomb gauge, the vector potential for such solutions reads

\[
\mathbf{A}^p(\mathbf{r}) = \mathbf{e}_{k\Lambda} e^{ik_z z}, \quad \mathbf{e}_{k\Lambda} \cdot \mathbf{k} = 0,
\]

(16)

where the vector \( \mathbf{e}_{k\Lambda} \) characterizes the photon with a certain helicity \( \Lambda = \pm 1 \), i.e. the photon’s spin projection onto its own momentum \( \mathbf{k} \). In the general case, when \( \mathbf{k} \) does not coincide with the quantization (\( z \)-axis) of the overall system and is given by equation (13), we can write the polarization vector \( \mathbf{e}_{k\Lambda} \) in the form

\[
\mathbf{e}_{k\Lambda} = -\frac{\Lambda}{\sqrt{2}} \left( \cos \theta k \cos \phi_{\Lambda} - i\Lambda \sin \theta k \sin \phi_{\Lambda} + i\Lambda \cos \phi_{\Lambda} \right).
\]

(17)

For practical applications, it is often convenient to present this vector as an expansion

\[
\mathbf{e}_{k\Lambda} = \sum_{m=0,\pm 1} c_m e^{im\phi_{\Lambda}} \eta_m,
\]

(18)

in the orthonormal basis \( \{\eta_m\}_{m=0,\pm 1} \) of the eigensolutions of the (\( z \)-component of) spin momentum operator:

\[
\hat{S}_z \eta_m = m \eta_m, \quad \eta_{\pm 1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm i \\ 0 \end{pmatrix}, \quad \eta_0 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}
\]

(19)

Moreover, the expansion coefficients in equation (18) are given by

\[
c_{\pm 1} = \frac{1}{2} \left( 1 \pm \Lambda \cos \theta \right), \quad \frac{\Lambda}{\sqrt{2}} \sin \theta k.
\]

(20)

Based on the decomposition (18), one can easily prove that the polarization vector \( \mathbf{e}_{k\Lambda} \) is an eigenfunction of the operator \( \hat{J}_z \) corresponding to the eigenvalue zero:

\[
\hat{J}_z \mathbf{e}_{k\Lambda} = \hat{L}_z \mathbf{e}_{k\Lambda} = \sum_{m=0,\pm 1} (-m + m) c_m e^{im\phi_{\Lambda}} \eta_m = 0.
\]

(21)

Here, we employed equation (19) and the trivial relation \( \hat{L}_z e^{-im\phi_{\Lambda}} = -m e^{-im\phi_{\Lambda}} \) written in the momentum space, where \( \hat{L}_z = -i \frac{\partial}{\partial \chi} \).

2.3. Vector potential of twisted states and its properties

Having discussed the orbital and the spin properties of the twisted-light solutions, we are now ready to write their explicit form. That is, the vector potential of the Bessel states can be expanded into plane waves as

\[
\mathbf{A}_{sk,m\Lambda}(\mathbf{r}) = A^p(\mathbf{r}) = \int a_{skm}(k_z) \mathbf{e}_{k\Lambda} e^{ik_z z} d^2k_z = \int a_{skm}(k_z) \mathbf{e}_{k\Lambda} e^{i(k_z r + k_z z)} d^2k_z
\]

(22)
As seen from this expression and equation (12), \( A_{k_{z},m_{x}}(\mathbf{r}) \) characterizes light with certain longitudinal \((k_{z})\) and transverse \((x)\) components of the linear momentum, as is requested by equations (4), (5) and (8). Moreover, since the product of the \( a_{x_{m}}(\mathbf{k}_{\perp}) \) and the polarization vector \( \mathbf{e}_{\Lambda} \) is an eigenfunction of the \( z\)-component of the TAM operator
\[
\hat{L}_{z} a_{x_{m}}(\mathbf{k}_{\perp}) \mathbf{e}_{\Lambda} = m_{z} a_{x_{m}}(\mathbf{k}_{\perp}) \mathbf{e}_{\Lambda},
\] (23)
as follows from equations (14) and (21) written in the momentum space, the requirement (6) is also fulfilled.

Equation (22) provides the most general form of the vector potential of the twisted (Bessel) states and will be employed in the following sections to explore the angular distribution of the emitted photoelectrons. Before we start with such an analysis, let us discuss first some basic properties of the twisted-light solutions. For example, by substituting the polarization vector \( \mathbf{e}_{\Lambda} \) in equation (22) and performing the integration over the transverse photon momentum \( \mathbf{k}_{\perp} \), we can write the vector potential \( \mathbf{A}^{w}(\mathbf{r}) \) in terms of eigenfunctions (19) of the spin operator \( \hat{S}_{z} \) as
\[
\mathbf{A}^{w}(\mathbf{r}) = \sum_{m_{\gamma}=0,\pm 1} \eta_{m_{\gamma}} \mathbf{A}^{w}_{m_{\gamma}}(\mathbf{r}),
\] (24)
where the coefficients \( \mathbf{A}^{w}_{m_{\gamma}}(\mathbf{r}) \) are given by
\[
\mathbf{A}^{w}_{m_{\gamma}}(\mathbf{r}) = \frac{1}{\sqrt{2\pi}} (\Pi)^{m_{\gamma}} c_{m_{\gamma}} J_{m_{\gamma}}(\chi r_{L}) e^{i(m_{\gamma} - m_{r})\varphi} e^{ik_{z}z}.
\] (25)
As seen from this expression, the potential \( \mathbf{A}^{w}(\mathbf{r}) \) is a superposition of three terms with different projections of the OAM \((m_{\gamma}=m_{\gamma}-m_{r})\) as well as SAM \((m_{r})\). The projection of the TAM for each term is then given by \( m_{r}\parallel+m_{r}=m_{r}\). Therefore, \( \mathbf{A}^{w}(\mathbf{r}) \) also possesses a projection of the TAM of \( m_{r} \) as required by constraint (6).

One may further simplify equations (24) and (25) if one assumes that the transverse momentum of the photon is much smaller comparing to its longitudinal momentum, \( x \ll k_{z} \). Within such a paraxial approximation, the summation in equation (24) is restricted to the single term \( m_{\gamma} = \Lambda \):
\[
\mathbf{A}^{w}(\mathbf{r}) = \eta_{\Lambda} \mathbf{A}^{w}_{\Lambda}(\mathbf{r})
= \eta_{\Lambda} \frac{1}{\sqrt{2\pi}} (\Pi)^{\Lambda} c_{\Lambda} J_{\Lambda}(\chi r_{L}) e^{i(\Lambda-m_{r})\varphi} e^{ik_{z}z}.
\] (26)
Equation (26) indicates that the projections of the orbital and spin angular momenta onto the \( z\)-axis decouple within the paraxial approximation, i.e.
\[
\hat{L}_{z} \mathbf{A}^{w}(\mathbf{r}) = (m_{r}\parallel-\Lambda) \mathbf{A}^{w}(\mathbf{r}), \quad \hat{S}_{z} \mathbf{A}^{w}(\mathbf{r}) = \Lambda \mathbf{A}^{w}(\mathbf{r}).
\] (27)
Moreover, in the limit \( \chi \to 0 \), where \( J_{\Lambda}(\chi r_{L}) \to \delta_{m_{\gamma},\Lambda} \), equation (26) recovers the standard solution for a plane wave that propagates along the \( z\)-axis.

3. Geometry of the photoionization process

3.1. Poynting vector and intensity profile of twisted light

To properly describe the geometry of the electron emission following the ionization of atoms by twisted waves, the spatial features of such waves have to be discussed. An appropriate quantity to characterize the spatial properties is given by the beam’s (time-averaged) Poynting vector [41] that is defined via
\[
\mathbf{P}(\mathbf{r}) = g_{P} \text{Re}[i \mathbf{A}^{w}(\mathbf{r}) \times (\nabla \times \mathbf{A}^{w}(\mathbf{r}))^{*}],
\] (28)
where \( g_{P} \) is a proportionality constant. By employing equation (20) as well as the decomposition (24) and, furthermore, using (local) basis vectors of the cylindrical coordinate system
\[
\mathbf{e}_{r} = \left( \cos \varphi, \sin \varphi, 0 \right), \quad \mathbf{e}_{\varphi} = \left( -\sin \varphi, \cos \varphi, 0 \right), \quad \mathbf{e}_{z} = \left( 0, 0, 1 \right),
\] (29)
one may write the Poynting vector (cf equation (13) in [36]) as
\[
\mathbf{P}(\mathbf{r}) = P_{r}(\mathbf{r}) \mathbf{e}_{r} + P_{\varphi}(\mathbf{r}) \mathbf{e}_{\varphi} + P_{z}(\mathbf{r}) \mathbf{e}_{z}
\] (30)
with
\[
P_{r}(\mathbf{r}) = 0,
\] (31)
\[
P_{\varphi}(\mathbf{r}) = g_{P} \frac{\chi^{2}}{2\pi} J_{m_{r}}(\chi r_{L}) (c_{1} J_{m_{r}}(\chi r_{L}) + c_{-1} J_{m_{r}+1}(\chi r_{L})),
\] (32)
and
\[
P_{z}(\mathbf{r}) = g_{P} \frac{\chi k}{2\pi} (c_{1} F_{m_{r}}(\chi r_{L}) - c_{-1} F_{m_{r}+1}(\chi r_{L})).
\] (33)
As seen from equations (30)–(33), no radial component of the Poynting vector is present and, therefore, we recover the well-known property that the Bessel beams are non-diffractive [42]. Furthermore, by taking the norm of the \( z\)-component of the Poynting vector, we derive the intensity profile of the Bessel beam within the plane that is perpendicular to the beam direction (\( z\)-axis) as
\[
I_{\perp}(\mathbf{r}) = |P_{z}(\mathbf{r})|^{2}.
\] (34)
From equations (33) and (34), one can deduce that the (transverse) intensity profile \( I_{\perp}(\mathbf{r}) \) has a pronounced radial structure that is given by the squared Bessel functions \( J_{m_{r}}^{2}(\chi r_{L}) \) with \( n = m_{r} - 1, m_{r} + 1 \), but is independent, however, of \( \varphi \). In figure 1, we display, for example, such an intensity pattern for the parameters that will be used in our photoionization calculations below and are summarized in the second column of table 1. At the centre of the figure, one can clearly see a zero-intensity spot (also called vortex) which is typical for beams that carry OAM [20–22]. This beam centre is surrounded by concentric rings of high and low intensities that alternate on a length scale of approximately \( 10^{4} \text{ au} \). As will be shown in the following section, such a pronounced structure of the Bessel solutions in contrast to the plane waves leads to a much more complex geometry of the atomic photoionization process.

3.2. Characterization of the electron emission

In order to explore the atomic photoionization, we shall first agree about the geometry and coordinates under which the electron emission is observed. Before starting such a discussion for the twisted waves, with their pronounced structure (cf figure 1), let us briefly recall how one
one can utilize this structure to define the well-defined (zero intensity) centre can be observed. Here, the typical ring structure of the intensity pattern with a pronounced structure of its electron cloud, such as the chosen arbitrarily. In contrast, for an atomic state which has a and y-axes are not predefined by the photon–atom system and can be adopted arbitrarily. A single polar angle \( \theta_p \) is needed in this case to characterize the emitted electron. If, in contrast, the atom was prepared before the ionization in the excited \( p_y \)-state, in which the electron density is not spherically symmetric but oriented along some preferred direction, we can employ this direction to define the y-axis.

As mentioned already, the Bessel waves—in contrast to plane wave photons—have a pronounced spatial profile which implies a more complex geometry of the ionization process. Apart from the z-axis which is chosen similar to before along the direction of the wave propagation, the x–z (reaction) plane has to be introduced. The plane passes through the position of the atom and the zero-intensity line as shown in figure 3. Therefore, except for the case when the atom is located just at the centre of the wave front, the emission of the electron following the ionization by twisted light is described by two angles \( \hat{n}_p = (\theta_p, \phi_p) \). The dependence of the differential (ionization) cross-section on these two angles will be studied below for different distances between the atom and the zero-intensity line as characterized by the impact parameter \( b \).

4. Angular distribution of the photoelectrons

Having discussed the vector potential of the twisted light and the geometry of the ionization process, we are now ready to study the angular distribution of the emitted electrons. Again, we start this investigation from the simple case of incident plane waves. Then, by analogy with the well-established plane wave treatment, we will lay down a general formalism for the description of the atomic ionization by Bessel beams.

### Table 1. Parameters of the twisted Bessel light used in the photoionization calculation.

| Light parameter | First scenario | Second scenario | Third scenario |
|-----------------|----------------|----------------|---------------|
| Photon energy \( E_p \) | 100 eV | 100 eV | 100 eV |
| Longitudinal momentum \( k_z \) | \( 2.68 \times 10^{-2} \) au | \( 2.67 \times 10^{-2} \) au | \( 1.89 \times 10^{-2} \) au |
| Transversal momentum \( x \) | \( 2.68 \times 10^{-4} \) au | \( 2.67 \times 10^{-4} \) au | \( 1.89 \times 10^{-4} \) au |
| Opening angle \( \theta_0 \) | 0.57° | 5.71° | 45° |
| Ratio \( s = x/k_z \) | 0.01 | 0.1 | 1 |
| Helicity \( \Lambda \) | +1 | +1 | +1 |
| \( \hat{z} \)-component of TAM \( m_{1p} \) | +3 | -3 | +3 |
4.1. Atomic ionization by plane wave photons

Not much has to be said about the theoretical description of the ionization of one-electron ions by plane wave photons. Within the first-order perturbation theory, any analysis of this process can be traced back to the evaluation of the matrix element

\[ M^{\text{pl}}_{fi}(\theta_p, \varphi_p) = \int \psi_f^*(r) \mathbf{A}^{\text{pl}}(r) \cdot \hat{p} \psi_i(r) \, d^3r, \]  

(35)

which describes the transition between the initial (bound) and final (continuum) electron states under the absorption of light whose properties are characterized by the vector potential (16). In equation (35), moreover, \( p \) is the electron momentum operator and the dependence of the transition amplitude on the electron emission angles \( (\theta_p, \varphi_p) \) results from the continuum wavefunction.

As can be seen from equation (35), the calculation of the matrix element \( M^{\text{pl}}_{fi} \) requires the knowledge of the bound—as well as continuum—state wavefunctions. Since in this work we aim to explore the (photoelectron) emission patterns for different shapes of the electron cloud in the initial atom, \( \psi_i(r) \) will be taken below as (i) the well-known Schrödinger solution

\[ \psi_i(r) \equiv \psi_{nlm}(r) = R_{nl}(r) Y_{lm}(\theta, \varphi), \]  

(36)

characterized by the principal quantum number \( n \), the OAM \( l \) and its projection \( m \) onto the \( z \)-axis and (ii) the wavefunction of the \( 2p_\text{p} \) level

\[ \psi_f(r) \equiv \psi_{p_\text{p}}(r) = \frac{1}{2i}(\psi_{2,1,+1}(r) + \psi_{2,1,-1}(r)). \]  

(37)

While the function \( \psi_{p_\text{p}}(r) \) characterizes a state whose electron density is oriented along the \( y \)-axis, the density \( \rho_{nlm}(r) = |\psi_{nlm}(r)|^2 \) of the state (36) is axially symmetric around the \( z \)-axis [43].

The final-state electron is described in our investigation by a plane wave

\[ \psi_f(r) \equiv \psi_{p_\text{p}}(r) = e^{i\mathbf{p} \cdot \mathbf{r}}, \]  

(38)

which constitutes the well-known Born approximation [44]. Within such an approximation that is valid for (electron) kinetic energies much larger than the ionization threshold, one neglects the electron–ion attraction after the ionization process. The great advantage of the approximation (38) is that it allows for a simple analytical evaluation of the transition amplitude \( M^{\text{pl}}_{fi}(\theta_p, \varphi_p) \). By inserting, for example, wavefunctions (36) and (38) into equation (35), we find

\[ M^{\text{pl}}_{fi}(\theta_p, \varphi_p) \equiv M^{\text{pl}}_{nlm}(\theta_p, \varphi_p) = (\mathbf{q} \cdot \mathbf{p}) \int e^{-i\mathbf{p} \cdot \mathbf{k} \cdot \mathbf{r}} \psi_{nlm}(\mathbf{r}) \, d^3\mathbf{r} \]

\[ = (2\pi)^3/2 (\mathbf{q} \cdot \mathbf{p}) \tilde{\psi}_{nlm}(\mathbf{q}), \]  

(39)

where \( \mathbf{q} \equiv \mathbf{p} - \mathbf{k} \) and the explicit form of the Fourier transform \( \tilde{\psi}_{nlm}(\mathbf{q}) \) is given in appendix A. With the help of this expression, moreover, one can immediately construct the ionization amplitude for the \( p_\text{y} \) state (37) as

\[ M^{\text{pl}}_{fi}(\theta_p, \varphi_p) \equiv M^{\text{pl}}_{p_\text{y}}(\theta_p, \varphi_p) \]

\[ = \frac{1}{2i} \left( M^{\text{pl}}_{2,1,+1}(\theta_p, \varphi_p) + M^{\text{pl}}_{2,1,-1}(\theta_p, \varphi_p) \right). \]  

(40)

In section 5, we will employ the matrix elements (39) and (40) in order to calculate the angular distribution of the emitted photoelectrons. Such a distribution is just given by the square of the amplitude

\[ W^{\text{pl}}(\theta_p, \varphi_p) = N^{\text{nlm}} |M^{\text{pl}}_{fi}(\theta_p, \varphi_p)|^2, \]  

(41)

where \( N^{\text{nlm}} \) is a normalization factor whose choice will be discussed later.

4.2. Atomic ionization by twisted photons

Similar to the plane wave case from above, we start the treatment of the atomic ionization by twisted Bessel photons with the discussion of the transition amplitude

\[ M^{\text{tw}}_{fi}(\theta_p, \varphi_p) = \int \psi_f^*(r) (\mathbf{A}^{\text{tw}}(r) \cdot \hat{p}) e^{-ib\mathbf{r} \cdot \mathbf{r}} \psi_i(r) \, d^3r. \]  

(42)

Again, \( \psi_i \) and \( \psi_f \) denote here the initial (bound) and final (continuum) electron wavefunctions, given by equations (36)–(38), correspondingly. Moreover, the vector potential of the incident twisted light is defined by expression (22), and the additional operator \( e^{-ib\mathbf{r} \cdot \mathbf{r}} \) translates the bound-electron wavefunction from the centre of the beam

\[ e^{-ib\mathbf{r} \cdot \mathbf{r}} \psi_i(r) = \psi_i(r - \mathbf{b}), \]  

(43)

thus incorporating the impact parameter of the atom with respect to the zero-intensity line (cf figure 3).

As for the evaluation of the plane wave matrix element (39), we can further simplify equation (42) if we employ the Fourier transformation of the bound-state wavefunction (36):

\[ M^{\text{tw}}_{fi}(\theta_p, \varphi_p) \equiv M^{\text{tw}}_{nlm}(\theta_p, \varphi_p) \]

\[ = (-i)^m \sqrt{\frac{\pi}{\kappa_1^3}} \int_0^{2\pi} e^{i\mathbf{m} \cdot \mathbf{q}} e^{-ib\mathbf{q} \cdot (\mathbf{e}_k \cdot \mathbf{p})} \tilde{\psi}_{nlm}(\mathbf{q}) \, d\mathbf{q}. \]  

(44)

By making use of the residue theorem from complex variable theory [45], the integral over the azimuthal angle \( \psi_\varphi \) in equation (44) can be calculated analytically. However, since the resulting expression is rather lengthy, we will not present it here and refer the interested reader to appendix B.

In a full analogy with equation (41), the square of the transition amplitude (42) describes—up to some normalization factor and within the non-relativistic framework—the angular distribution of the electrons emitted due to atomic ionization by twisted Bessel light. This angular distribution is obtained for the case when the vector potential \( \mathbf{A}^{\text{tw}}(r) \) describes the most general solutions of the vector Helmholtz equation that have a well-defined projection of the TAM onto the \( z \)-direction. Our analysis goes, therefore, beyond the paraxial approximation in contrast to previous photoionization studies [32, 33]. In the following section, we apply the derived formalism to investigate the electron emission from different bound states of a neutral hydrogen atom.

5. Results and discussion

In the previous section, we have laid out a general formalism for the description of the angular distribution of electrons emitted in the ionization of hydrogen-like systems by twisted Bessel light. While, of course, this theory can be applied to the photoemission from any (one-electron) bound state,
we first focus our analysis on the K-shell ionization of a neutral hydrogen atom. Furthermore, we have to agree on the properties of the twisted photon beam. In our calculations, we will describe this beam by either of three different sets of beam parameters that are summarized in Table 1. For all scenarios described in Table 1, the energy of the incident light is chosen to be \( E_p = \omega = 100 \text{ eV} \), that—being well above the 1s ionization threshold—ensures the validity of the Born approximation (38). Moreover, twisted photons within this energy range have been recently produced by utilizing a helical undulator at the synchrotron light source BESSY II [46].

Having defined the prerequisites, let us now discuss the ionization process for the scenario that is characterized by the second column of Table 1. Here, the ratio of transverse to longitudinal components of the photon’s linear momentum, \( s = \frac{\omega}{k} \), amounts to \( s = 0.01 \) which lies well within the region of the paraxial approximation (26). The electron emission pattern evaluated for such a set of parameters is presented for different impact parameters \( b \), that characterize the position of the atom in the wavefront (cf. Figure 3), and three polar angles \( \theta_p = 45^\circ \) (left panel), \( \theta_p = 60^\circ \) (middle panel) and \( \theta_p = 90^\circ \) of the (continuum) electron. For comparison, the emission pattern predicted for the incoming plane wave photons with helicity \( \Lambda = +1 \) is depicted by the dashed line.

As can be seen from Figure 4, the angular distribution \( W^\text{tw}(\theta_p, \varphi_p) \) is isotropic if the atom is placed at the centre of the wavefront. This is well expected since the system of ‘atom in the 1s state + Bessel beam’ possesses for \( b = 0 \) cylindrical symmetry about the \( z \)-axis and, hence, the photoionization probability is independent on the azimuthal angle. Such a symmetry is broken if one shifts the atom position from the zero-intensity centre. A remarkable anisotropy of the electron emission pattern can be observed, therefore, for impact parameters in the range \( 0 < b \lesssim 100 \text{ au} \). However, if the distance between the atom and the wavefront becomes very large, \( b > 100 \text{ au} \), the angular distribution \( W^\text{tw}(\theta_p, \varphi_p) \) converges to the one that results from the plane wave photoionization. Such an impact parameter behaviour can be easily understood if one compares the characteristic scales of the atomic target and the Bessel beam. Namely, while the intensity profile of the light front changes notably on a length scale of \( 10^5 \text{ au} \) (see Figure 1), the ground-state electron is confined to a volume characterized by a linear size of a few atomic units. Therefore, the electron does not ‘see’ the large-scale (radial) variations of the light intensity profile, and its emission can be affected only by the phase structure of the Bessel photons as defined by the terms \( e^{im\varphi_p} \) in equations (24) and (25). Obviously, the change of this phase structure on the scale of an atomic Bohr radius can be remarkable only for relatively small parameters \( b \). In contrast, far away from the light-wave axis, the \( e^{im\varphi_p} \) term varies slowly over the extension of the atom and the electron cloud is exposed to an (almost) constant phase. For \( b > 100 \text{ au} \), therefore, the ionization by twisted light resembles the one by plane wave photons as one may observe in Figure 4. Moreover, we would like to note that since the electron distribution within the paraxial regime is seen to depend solely on the phase structure of the incoming Bessel beam, it is expected that the same results as presented here hold also true for a (paraxial) Laguerre–Gaussian beam with the same OAM and whose parameters are chosen such that its intensity profile varies slowly over the extension of the atom.

We note here that in the previous scenario, we analysed the angular distribution of the emitted electrons only for the fixed value \( m_p = 3 \) of the photon’s TAM. To investigate the effect of varying \( m_p \), we display in Figure 5 the electron distribution for the same beam parameters as before but with

![Figure 4](image-url)
different values of $m_\gamma$ and for different impact parameters $b$. As seen from the figure, the effect on the emission pattern by changing the TAM is significant only for relatively small impact parameters, and becomes negligible for larger ones. This behaviour should be clear from our discussion above: the influence of the photon’s TAM $m_\gamma$ (incorporated by the phase factor $e^{im_\gamma \phi}$) can be large only for atoms that are positioned near the beam axis. A strong dependence of the electron distribution on $m_\gamma$ is, therefore, seen for atoms with relatively small impact parameters, whereas atoms that are far away from the beam axis do not ‘feel’ the change of the TAM.

Until now we have discussed the impact parameter dependence of the angular distribution $W^{tw}(\theta_p, \phi_p)$ for the parameters of the incident light given in the second column of table 1. In particular, we have restricted our analysis to the case where the transversal component $\chi$ of the photon’s linear momentum is negligible with respect to the longitudinal component $k_z$. In order to understand how the electron emission pattern changes if one departs from such a paraxial approximation, calculations have been performed for the same photon energy and helicity as before but for three different values of the parameter $s = \chi/k_z$: $s = 0.01$, $s = 0.1$ and $s = 1$ (cf table 1). While the first of these values obviously corresponds to the paraxial limit, the last one describes the general (non-paraxial) regime. In figure 6, we display the angular distribution $W^{tw}(\theta_p, \phi_p)$ that has been evaluated for these $s$ values as well as for the impact parameters $b = 100$ au (left panel), $b = 1000$ au (middle panel) and $b = 10\,000$ au (right panel). As can be seen from the figure, the electron emission pattern appears to be very sensitive to the variation of $s$. That is, while $W^{tw}(\theta_p, \phi_p)$ is almost isotropic in the paraxial regime ($s = 0.01$), it shows a remarkable $\phi_p$-dependence if the transversal component of the photon linear momentum is comparable to the longitudinal one ($s \sim 1$). In order to understand this sensitivity to the component ratio $s$, one has to revisit equation (34), which describes the intensity profile of the twisted wavefront. This equation suggests that
the length scale of the intensity oscillations depends—via the squares of the Bessel functions—on the value of the transversal momentum. For large \( k_z \) and, hence, \( s \sim 1 \), the period of oscillations is of the length scale of 100 au and becomes comparable with the size of the atomic ground state. The electron wavefunction may ‘feel’, therefore, the features of the intensity distribution of the photon beam and this is reflected in the angular distribution as shown in figure 6.

The 1s-ground state of the hydrogen atom, whose ionization has been discussed so far, possesses spherical symmetry. The \( \varphi_p \)-dependence of the photoelectron emission pattern was caused, therefore, by the displacement of the target atom with respect to the zero-intensity centre of the wavefront. Apart from such a displacement, one can break the cylindrical symmetry of the overall system ‘target + incident light’ if one prepares the initial atom in some oriented state. In this work, for example, we investigated the ionization of the hydrogenic 2p state (37) by twisted light that is characterized by the parameters given in the second column of table 1. The angular distribution \( W^{tw} (\theta_p, \varphi_p) \), computed for these parameters and for different positions of the atom within the wavefront, is displayed in figure 7 as a function of the azimuthal angle \( \varphi_p \). As expected from the discussion of the symmetry properties of the 2p state, the \( W^{tw} (\theta_p, \varphi_p) \) is remarkably anisotropic even at zero impact parameter. With the increase of \( b \), the shape of the angular distribution varies significantly until it resembles—for \( b > 100 \text{ au} \)—the emission pattern of the electrons emitted in the atomic ionization by plane wave photons (cf figure 7). This impact parameter behaviour can be explained by the same reasoning as given for the K-shell ionization.

As can be seen from figures 4–7, a pronounced \( \varphi_p \)-behaviour of the electron angular distribution \( W^{tw} (\theta_p, \varphi_p) \) that is attributed to the phase structure (paraxial regime) or to the intensity profile (non-paraxial regime) of the twisted waves can be observed for impact parameters in the range \( 0 < b < 100 \text{ au} \) and \( 0 < b < 10000 \text{ au} \), respectively. The experimental measurement of the predicted effects would require, therefore, an operational control of the parameter \( b \). Even though the practical realization of such a control is a very complicated task, the recent advances in atomic trap technologies suggest that it might become feasible in the near future. For example, it is currently feasible to trap an atom with a spatial uncertainty of several nm [47–49], which is just of the order where the characteristic photoionization features of the Bessel beams become visible (cf figure 6).

6. Summary and outlook

In this work, we have performed a theoretical analysis of the atomic ionization by twisted (Bessel) photons. By making use of the non-relativistic Schrödinger theory and the first-order perturbative approach, we laid down a general formalism for the description of the photoelectron angular distribution. While this theory can be employed to analyse the ionization of an arbitrary hydrogenic level, detailed calculations have been performed for the electron emission from the 1s ground and 2p excited states. Our results indicate that the emission pattern is very sensitive to the position of the target atom within the wave as characterized by the impact parameter \( b \) with respect to the zero-intensity wavefront centre. For relatively small impact parameters, \( b \lesssim 100 \text{ au} \) for the paraxial and \( b \lesssim 10000 \text{ au} \) for the non-paraxial light beams, the electron angular distribution reflects the phase structure and the intensity profile of the Bessel solutions, respectively. In contrast, if the atom is displaced far away from the beam centre, the electron emission remains almost unaffected by the intensity and phase structure of the twisted beam and resembles the one that is observed for the ionization by plane waves.

Our present study provides a theoretical basis for the analysis of the atomic photoeffect in the most general case, i.e. it is not restricted to the paraxial regime of the (twisted) light propagation. It complements, therefore, previous photoionization studies [32, 33] and opens up a way for further and deeper investigations of the ionization properties. In particular, by making use of the derived expressions, we aim to explore the ionization of Rydberg atoms and to analyse the OAM states of the emitted photoelectrons. This will help to clarify the question whether and how the...
photoeffect can be employed for the production of twisted electrons. Moreover, the developed analytical approach can be extended to study other fundamental processes, such as, for example, photo-excitation, photo-emission and photon scattering of twisted photons as well as elastic scattering of twisted electrons by atoms and ions. Such investigations are of special importance in the field of quantum computing (as noted by [50]), where twisted particles could lead to an improvement of the OAM transfer between quantum systems. Intensive theoretical analysis of atomic processes with twisted particles is therefore required and additional studies are currently underway.

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Appendix A. Fourier transform of the bound-state wavefunction

As can be seen from equations (35) and (39), the evaluation of the amplitude for the bound-free electron transition under the absorption of the plane wave photons can be traced back to the Fourier transform of the wavefunction (36). Within the non-relativistic framework, this transform reads as [51, 52]

\[ \tilde{\psi}_{nlm}(\mathbf{p}) = \frac{2^{l+1} l!}{(2\pi)^2} \frac{1}{\sqrt{Z(n+l)!}} \left( \frac{p}{Z} \right)^l \times \frac{Z^{2l+4}}{(p^2 + \delta^2)^{l+2}} C_{n-l-1}^{l+1} \left( \frac{p^2 - \delta^2}{p^2 + \delta^2} \right) Y_{lm}(\theta, \varphi, p), \]  

(A.1)

where \( \delta = Z/n \) with the nuclear charge \( Z \) and \( C_{n-l-1}^{l+1}(x) \) is a so-called Gegenbauer polynomial [40].

Appendix B. Matrix elements for photoionization by twisted photons

Similar to the ionization by plane wave photons, any analysis of the electron emission induced by the incident twisted light requires the knowledge of the transition amplitude (42). As discussed in section 4.2, this amplitude can be written, upon the Fourier transformation of the bound-state wavefunction, in the form of (44). In order to proceed further, we insert the explicit expression (A.1) of \( \tilde{\psi}_{nlm}(\mathbf{q}) \) into equation (44) and find

\[ M_{nlm}^{tw}(\theta_p, \varphi_p) = c_{tw} \int_0^{2\pi} e^{im_\psi_p} e^{-ibq_\psi} \left( \frac{\mathbf{e}_\lambda \cdot \mathbf{p}}{q^2 + \delta^2} \right)^l \times C_{n-l-1}^{l+1}(\frac{q^2 - \delta^2}{q^2 + \delta^2}) Y_{lm}(\theta_q, \varphi_q) d\psi_k, \]  

(B.1)

where \( \mathbf{q} = \mathbf{p} - \mathbf{k} \) and the prefactor \( c_{tw} \) is given by

\[ c_{tw} = (-i)^{m_\psi_p+l} 2^{l+2} n^{-l-2} Z^{2l+4} \times \frac{2\pi(n-l-1)!}{\pi Z^2(n+l)!}. \]  

(B.2)

It follows from these formulas that the computation of the transition amplitude \( M_{nlm}^{tw}(\theta_p, \varphi_p) \) is reduced to an integration over the azimuthal angle \( \varphi_k \). To perform such an integration analytically, we need to re-write the integrand on the right-hand side of equation (B.1) in such a way that its \( \varphi_k \)-dependence becomes explicit. We start from the product of the polarization \( \mathbf{e}_\lambda \) and the momentum \( \mathbf{p} \) vectors which can be simplified to

\[ (\mathbf{e}_\lambda \cdot \mathbf{p}) = \frac{p_+}{\sqrt{2}} c_{-1} e^{i(\varphi_+ - \varphi_-)} + p_- c_0 - \frac{p_+}{\sqrt{2}} c_{+1} e^{-i(\varphi_+ - \varphi_-)} \]  

(B.3)

with

\[ p_+ = p \sin \theta_p, \quad p_- = p \cos \theta_p. \]  

(B.4)

As a second step, we shall expand the spherical harmonics \( Y_{lm}(\theta_q, \varphi_q) \) in terms of \( Y_{\sigma \mu}(\theta_k, \varphi_k) \). To perform this expansion, we introduce the solid spherical harmonics:

\[ R_{lm}(\mathbf{r}) = \frac{4\pi}{2l+1} Y_{lm}(\theta, \varphi), \]  

(B.5)

for which the following addition theorem [53] holds:

\[ R_{lm}(\mathbf{r} + \mathbf{a}) = \sum_{\sigma=0}^{2l} \sum_{\mu=-\sigma}^{\sigma} \left( \frac{2l+1}{2\sigma} \right)^{1/2} \times (\sigma, \mu; l - \sigma, m - \mu |lm) R_{\sigma \mu}(\mathbf{r}) R_{l - \sigma, m - \mu}(\mathbf{a}). \]  

(B.6)

By re-writing the spherical harmonics \( Y_{l - \sigma, m - \mu}(\theta_k, \varphi_k) \) in this expression in terms of \( e^{im_\psi_p} \), we obtain

\[ \tilde{\psi}_{nlm}^{tw}(\mathbf{q}) = \int \frac{2l+1}{4\pi} R_{lm}(\mathbf{q}) \]  

\[ \tilde{\psi}_{nlm}^{tw}(\mathbf{q}) = \sum_{\sigma=0}^{2l} \sum_{\mu=-\sigma}^{\sigma} h_{\sigma \mu}(\theta_p, \varphi_p) e^{i(m_\psi_p \varphi_k)} \]  

(B.10)

with

\[ h_{\sigma \mu}(\theta_p, \varphi_p) = \sqrt{\frac{2l+1}{2\sigma+1}} \left( \frac{(l - \sigma + m - \mu)!}{(l - \sigma - m - \mu)!} \right)^{1/2} \times Y_{\sigma \mu}(\theta_p, \varphi_p) R_{l - \sigma, m - \mu}(\mathbf{cos} \theta_k). \]  

(B.11)

Having deduced the explicit \( \varphi_k \)-dependence of the product \( (\mathbf{e}_\lambda \cdot \mathbf{p}) \) and of the expression \( \tilde{\psi}_{nlm}^{tw}(\theta_q, \varphi_q) \) from equation (B.1), it remains to perform the Fourier expansion

\[ \frac{1}{(2\pi)^2} \int_0^{2\pi} e^{im_\psi_p} d\psi_k = \sum_{\nu=-\infty}^{\infty} f_\nu(\theta_p, \varphi_p) e^{i\nu \varphi_k}, \]  

(B.12)
of the Gegenbauer polynomial $C_{n-l-1}^{(l+1)}(x)$ divided by some polynomial. In order to compute the expansion coefficients

$$f_v(\theta_p, \varphi_p) = \frac{1}{2\pi} \int_0^{2\pi} \frac{1}{(q^2 + \delta^2)^{l+2}} \times C_{n-l-1}^{(l+1)} \left( \frac{q^2 - \delta^2}{q^2 + \delta^2} \right) e^{-i\varphi_k} \, d\varphi_k,$$

we write the Gegenbauer polynomials explicitly [40] as

$$C_{n-l-1}^{(l+1)} \left( \frac{q^2 - \delta^2}{q^2 + \delta^2} \right) = \sum_{n=0}^{(n-l-1)/2} t_n \left( \frac{q^2 - \delta^2}{q^2 + \delta^2} \right)^{n-l-1-2\eta},$$

where $[x]$ is the largest integer not greater than $x$ and

$$t_n = \frac{(n + \eta - 1)!}{\eta! \, (n - l - 1 - 2\eta)!}.$$  \hspace{1cm} (B.15)

By inserting equation (B.14) into (B.13), we find the Fourier expansion coefficients in the form

$$f_v(\theta_p, \varphi_p) = \frac{1}{2\pi} \sum_{n=0}^{(n-l-1)/2} \sum_{\eta=0}^{\min{(n, n-l-1)}} t_\eta \int_0^{2\pi} \varphi_k \left( \frac{q^2 - \delta^2}{q^2 + \delta^2} \right)^{n-l-1-2\eta} e^{-i\varphi_k} \, d\varphi_k.$$  \hspace{1cm} (B.16)

In order to compute the integral from above, we perform the substitution $\varphi_k = \varphi_p - \varphi_k$ and introduce the new (integration) variable

$$z = e^{i\varphi_k},$$

and, hence, re-write (B.16) as

$$f_v(\theta_p, \varphi_p) = \frac{-1}{2\pi} \alpha^{-l-2} e^{-i\varphi_p} \sum_{n=0}^{(n-l-1)/2} t_\eta \int_c g_{\nu}(z) \, dz.$$  \hspace{1cm} (B.18)

Here, the integration contour $\chi$ is the complex unit circle, and the function $g_{\nu}(z)$ is given by

$$g_{\nu}(z) = e^{i\nu+1} (z - z_1)^{n-l-1-2\eta} (z - z_2)^{n-l-1-2\eta} \times (z - z_3)^{-n-1+2\eta} (z - z_4)^{-n-1+2\eta},$$

with

$$\alpha = -p_\perp x,$$

and

$$z_1 = (2p_\perp x)^{-1} [p^2 + k^2 - \delta^2 - 2p_k k_z] + \sqrt{(p^2 + k^2 - \delta^2 - 2p_k k_z)^2 - 4p_\perp^2 x^2}],$$

$$z_2 = (2p_\perp x)^{-1} [p^2 + k^2 - \delta^2 - 2p_k k_z] - \sqrt{(p^2 + k^2 - \delta^2 - 2p_k k_z)^2 - 4p_\perp^2 x^2}],$$

$$z_3 = (2p_\perp x)^{-1} [p^2 + k^2 + \delta^2 - 2p_k k_z] + \sqrt{(p^2 + k^2 + \delta^2 - 2p_k k_z)^2 - 4p_\perp^2 x^2}],$$

and

$$z_4 = (2p_\perp x)^{-1} [p^2 + k^2 + \delta^2 - 2p_k k_z] - \sqrt{(p^2 + k^2 + \delta^2 - 2p_k k_z)^2 - 4p_\perp^2 x^2}.$$  \hspace{1cm} (B.24)

As can be seen from equation (B.19), the $g_{\nu}(z)$ is a rational function with poles at $z = 0$ and $z = z_4$ in the unit circle of order $-\nu - l - 1$ and $n + 1 - 2\eta$, respectively. We can use, therefore, the residue theorem [45] to calculate the integral over $z$ in equation (B.18) analytically

$$f_v(\theta_p, \varphi_p) = e^{-i\varphi_p} \alpha^{-l-2} \times \sum_{\eta=0}^{(n-l-1)/2} t_\eta \left( \text{Res}(g_{\nu}, 0) + \text{Res}(g_{\nu}, z_4) \right),$$

where

$$\text{Res}(g_{\nu}, z_\text{pole}) = \lim_{z\to z_\text{pole}} \frac{\delta^{k-1}}{\delta z^{k-1}} (z - z_\text{pole})^k g_{\nu}(z)$$

and $k$ is the order of the pole $z_\text{pole}$. By inserting the function $g_{\nu}(z)$ on the right-hand side of equation (B.26) and evaluating the derivative for the two poles $z = 0$ and $z = z_4$, we finally obtain

$$\text{Res}(g_{\nu}, 0) = \frac{1}{(-\nu - l - 2)!} \times \sum_{i_0=0}^{\nu-l-2} \sum_{i_1=0}^{l} \sum_{i_2=0}^{n-2\eta} \left( -\nu - l - 2 - i_0 \right) \left( -\nu - l - 2 - i_0 - i_1 \right) \left( -\nu - l - 2 - i_0 - i_1 - i_2 \right) \times (n - l - 1 - 2\eta) \times (n - l - 1 - 2\eta) \times (n - l - 1 - 2\eta) \times (n - l - 1 - 2\eta),$$(B.27)

and

$$\text{Res}(g_{\nu}, z_4) = \frac{1}{(n - 2\eta)!} \sum_{i_0=0}^{n-2\eta} \sum_{\nu-l-2} \sum_{i_1=0}^{l} \sum_{i_2=0}^{n-2\eta} \left( n - 2\eta \right) \times (n - 2\eta - i_0) \times (n - 2\eta - i_0 - i_1) \times (n - 2\eta - i_0 - i_1 - i_2) \times (n - l - 1 - 2\eta) \times (n - l - 1 - 2\eta) \times (n - l - 1 - 2\eta) \times (n - l - 1 - 2\eta),$$(B.28)

where $(x)_j = x(x-1)(x-2)\cdots(x-j)$ is the falling factorial. With the help of equations (B.25)–(B.28), one may evaluate the expansion coefficients $f_v(\theta_p, \varphi_p)$ that enter the Fourier expansion (B.12). Numerical analysis of these coefficients has shown, moreover, that for the ground and low-lying excited atomic states and for small photon energies ($\approx 100$ eV), the summation over $\nu$ in equation (B.12) may be restricted just to terms with $|\nu| \lesssim 3$.

After the separate evaluation of the three parts of the integrand in equation (B.1), we are now ready to compute the matrix element $M_{ji}^{\nu}(\theta_p, \varphi_p)$. That is, by inserting
equations (B.3), (B.10) and (B.12) in the right-hand side of equation (B.1), we find
\[
M_{ij}^{\text{tw}}(\theta_p, \varphi_p) = c_{ijw} \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \int_0^{2\pi} \tilde{h}_{\sigma \mu}(\theta_p, \varphi_p) f_i(\theta_p, \varphi_p) \times e^{i(m_p + m + \mu - \mu) \phi_k} e^{-ibq} \times \left( \frac{p_+}{\sqrt{2}} C_{-1} e^{-i(\phi_k - \phi_p)} + p_c \frac{p_0}{\sqrt{2}} C_{+1} e^{i(\phi_k - \phi_p)} \right) d\phi_k.
\]
We further utilize the well-known integral representation [40] of the Bessel functions
\[
\int_0^{2\pi} e^{i\psi} e^{i\psi \cos(\phi - \phi')} d\phi = 2\pi i e^{i\psi f_i(x)},
\]
to analytically perform the integration over the \( \varphi_k \)-angle in equation (B.29), and to yield finally the general expression
\[
M_{ij}^{\text{tw}}(\theta_p, \varphi_p) = 2\pi c_{ijw} \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \tilde{h}_{\sigma \mu}(\theta_p, \varphi_p) f_i(\theta_p, \varphi_p) \times e^{i(m_p + m + \mu - \mu) \phi_k} e^{-ibq} e^{i(m_p + m + \mu - \mu) \phi_k} \times \left( \frac{p_+}{\sqrt{2}} C_{-1} e^{-i(\phi_k - \phi_p)} f_i(m_p + m + \mu - \mu + 1) (\kappa b_{1}) \right. \\
\left. + p_c \cos m_p + m + \mu (\chi b_{1}) \right) + i \frac{p^1}{\sqrt{2}} C_{+1} e^{i(\phi_k - \phi_p)} f_i(m_p + m + \mu - \mu - 1)(\chi b_{1}) \right) \right)
\]
for the amplitude that describes the bound-free electron transition in the field of the twisted (Bessel) light. In this expression, \( \varphi_k \) is the azimuthal angle of the impact parameter, which should be taken to be zero for the geometry used in the present study (cf figure 3).

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