

Rotational effects of twisted light on atoms beyond the paraxial approximation

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The transition probability for the emission of a Bessel photon by an atomic system is calculated within first order perturbation theory. We derive a closed expression for the electromagnetic potentials beyond the paraxial approximation that permits a systematic multipole approximation. The matrix elements for the center of mass and internal motion are explicitly evaluated for some particularly relevant cases. This permits to clarify the feasibility of observing the rotational effects of twisted light on atoms predicted by the calculations. It is shown that the probability that the internal state of an atom acquires orbital angular momentum from light is, in general, maximum for an atom located at the axis of a Bessel mode. For a Gaussian packet, the relevant parameter is the ratio of the spread of the atomic center of mass wave packet to the transversal wavelength of the photon.

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I. INTRODUCTION

It is important to understand the influence of the angular momentum of light on the dynamics of atomic systems and microparticles from the point of view of basic and applied physics. The work by Beth [1] showed that circularly polarized light has rotational effects on rigid bodies. Likewise, observed atomic transitions are simply described in terms of the angular momentum carried by plane wave circularly polarized photons. Thus, the phenomenological relation between spin angular momentum and polarization is well established.

In the last few years it has been shown both theoretically [2] and experimentally [3] that light beams may carry angular momentum not directly related to their polarization state. This form of angular momentum is usually qualified as orbital and is due to an azimuthal phase dependence of the transverse electromagnetic intensity. For laser beams properly described within the paraxial approximation, e.g., Laguerre-Gaussian beams, the total angular momentum of light can be clearly divided into spin and orbital parts; this separation has direct physical consequences on the motion of microparticles [3,4]. In the case of atoms, the orbital angular momentum of paraxial light can induce torques in the center of mass [5,6] while the probability of changing the internal angular momentum is very small [6,8]. However, the separation between orbital and spin angular momentum is not so natural beyond the paraxial approximation [9,10]. On the one hand, the general forms of these quantities, as they usually appear in the literature, are not gauge invariant [11,12], despite the fact that physical observables are expected to be so. On the other hand, the concept of polarization for twisted light is not identical to that used for plane waves since, in general, the electric and/or magnetic field of twisted beams are nonzero along the main propagation axis.

Among electromagnetic modes carrying orbital angular momentum, Bessel modes are particularly interesting be-

cause they propagate with an intensity pattern invariant along its axis [13]. Experimental realizations of such beams and their mechanical effects on microparticles are the subject of many current investigations [4]. Studies concerning the separation between spin and orbit angular momentum have been carried out both semiclassically [14] and quantum mechanically [10,15]. The quantum dynamical properties of the Bessel photons should, in principle, be studied via the operators assigned to energy, momentum, orbital angular momentum, and spin using the standard quantum optics formalism. However, direct calculations show that these operators do not follow the algebra of the translation and rotation group [10,15]. Actually, the standard spin operator has a behavior more similar to an helicity operator.

The purpose of the present paper is to study in detail the rotational effects of Bessel photons on atomic systems. This is a dynamical mean to measure the mechanical properties of twisted light. To this end, we evaluate the transition amplitude for the spontaneous emission of a Bessel photon by a non relativistic hydrogenic atom within first order perturbation theory. In the next section, we describe the system including the interaction which is incorporated using minimal coupling in the Coulomb gauge. Then, an explicit expression relevant for a systematic multipole approximation is obtained and it is applied to the explicit calculation of matrix elements of the interaction Hamiltonian between an unperturbed atom and electromagnetic field states. Finally, a comparison with previous results is given, and some conclusions following our results are summarized.

II. THE ATOM-RADIATION SYSTEM

Consider two particles of opposite charges q_e and q_N , gyromagnetic ratios g_e and g_N , masses M_e and M_N , and vector positions \mathbf{r}_e and \mathbf{r}_N . This hydrogenlike atom is assumed to be described to a good approximation by a nonrelativistic Hamiltonian of the form

$$\hat{H}_P = \frac{p_e^2}{2M_e} + \frac{\hat{P}_N^2}{2M_N} + V_r + V_R, \quad (1)$$

with V_r an internal potential depending on the relative coordinate $\mathbf{r} = \mathbf{r}_e - \mathbf{r}_N$ and V_R an external potential that affects the

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center of mass coordinate $\mathbf{R}=(M_e\mathbf{r}_e+M_N\mathbf{r}_N)/(M_e+M_N)$. The atom state can be written as a superposition of wave functions

$$\Psi(\mathbf{r}_e, \mathbf{r}_N, \chi_e, \chi_N) = \Phi(\mathbf{R})\phi(\mathbf{r})\chi_N\chi_e e^{-iEt/\hbar}, \quad (2)$$

where

$$\left[\frac{p_{CM}^2}{2M} + V_R(\mathbf{R}) \right] \Phi(\mathbf{R}) = E_{CM}\Phi(\mathbf{R}), \quad (3)$$

$$\left[\frac{\hat{p}^2}{2\mu} + V_r(\mathbf{r}) \right] \phi(\mathbf{r}) = E_{rel}\phi(\mathbf{r}), \quad (4)$$

$$E = E_{CM} + E_{rel} \quad (5)$$

and χ_e, χ_N are the spinors associated to each particle. In the simplest case

$$V_r(\mathbf{r}_e - \mathbf{r}_N) = \frac{q_e q_N}{|\mathbf{r}_e - \mathbf{r}_N|} \quad (6)$$

and $V_R=0$.

We are interested in the perturbative description of the interaction of the atom with a Bessel mode. Thus, the quantization of the free radiation field will be done using transverse magnetic (TM) and transverse electric (TE) Bessel vector potentials; in the Coulomb gauge, they are given by

$$\mathbf{A}_\kappa^{(TM)} = \frac{c}{2\omega} E_0 e^{i(k_z z - \omega t)} \times \left(\psi_{m-1}(\mathbf{e}_x + i\mathbf{e}_y) - \psi_{m+1}(\mathbf{e}_x - i\mathbf{e}_y) - i \frac{2k_\perp}{k_z} \psi_m \mathbf{e}_z \right), \quad (7)$$

$$\mathbf{A}_\kappa^{(TE)} = \frac{i}{2k_z} E_0 e^{i(k_z z - \omega t)} [\psi_{m-1}(\mathbf{e}_x + i\mathbf{e}_y) + \psi_{m+1}(\mathbf{e}_x - i\mathbf{e}_y)], \quad (8)$$

where κ denotes the set of quantum numbers $\{k_\perp, k_z, m\}$,

$$\psi_m(\rho, \phi; k_\perp) = J_m(k_\perp \rho) e^{im\phi}, \quad (9)$$

J_m is the cylindrical Bessel function of order m ,

$$\omega = c\sqrt{k_\perp^2 + k_z^2} \quad (10)$$

and

$$E_0^2 = \frac{\hbar k_\perp}{2\pi} \left[\frac{k_z^2 c^2}{\omega} \right]. \quad (11)$$

The corresponding electric fields are $\mathbf{E}_\kappa^{(i)} = i\omega/c\mathbf{A}_\kappa^{(i)}$ while the magnetic fields are

$$\mathbf{B}_\kappa^{(TM)} = \frac{E_0 \omega}{2ck_z} e^{i(k_z z - \omega t)} [\psi_{m-1}(\mathbf{e}_x + i\mathbf{e}_y) - \psi_{m+1}(\mathbf{e}_x - i\mathbf{e}_y)], \quad (12)$$

$$\mathbf{B}_\kappa^{(TE)} = \frac{iE_0}{2} e^{i(k_z z - \omega t)} \times \left(\psi_{m-1}(\mathbf{e}_x + i\mathbf{e}_y) + \psi_{m+1}(\mathbf{e}_x - i\mathbf{e}_y) - i \frac{2k_\perp}{k_z} \psi_m \mathbf{e}_z \right). \quad (13)$$

From the electromagnetic potentials, the operator $\hat{\mathbf{A}}$ is obtained as

$$\hat{\mathbf{A}}(\mathbf{r}, t) = \sum_{i=TM, TE} \sum_{m=-\infty}^{\infty} \int_0^{\infty} dk_\perp \int_{-\infty}^{\infty} dk_z [\hat{a}_m^{(i)}(k_z, k_\perp) \mathbf{A}_\kappa^{(i)}(\mathbf{r}, t) + \hat{a}_m^{(i)\dagger}(k_z, k_\perp) \mathbf{A}_\kappa^{(i)*}(\mathbf{r}, t)], \quad (14)$$

$$[\hat{a}_m^{(i)}(k_z, k_\perp), \hat{a}_{m'}^{(i)\dagger}(k'_z, k'_\perp)] = \frac{1}{k_\perp} \delta_{m, m'} \delta(k_\perp - k'_\perp) \delta(k_z - k'_z). \quad (15)$$

The normalization condition imposed on the potentials (7) and (8) guarantees that the radiation energy operator can be written as [15]

$$\hat{H}_R = \sum_{i, m} \int dk_\perp dk_z \hbar \omega \hat{N}_m^{(i)}, \quad (16)$$

$$\hat{N}_m^{(i)} = \frac{1}{2} (\hat{a}_m^{(i)\dagger} \hat{a}_m^{(i)} + a_m^{(i)} \hat{a}_m^{(i)\dagger}).$$

The linear momentum electromagnetic operator is

$$\hat{\mathbf{P}} = \hbar \sum_i \int dk_\perp dk_z [k_\perp \hat{\Pi}_+^{(i)}(\mathbf{e}_x - i\mathbf{e}_y) + k_\perp \hat{\Pi}_-^{(i)}(\mathbf{e}_x + i\mathbf{e}_y) + k_z \hat{\Pi}_3^{(i)} \mathbf{e}_z], \quad (17)$$

where the operators $\hat{\Pi}_{\pm, 3}^{(i)}(k_\perp, k_z)$ are

$$\hat{\Pi}_+^{(i)} = i \sum_m \hat{a}_{m-1}^{(i)\dagger} \hat{a}_m^{(i)}, \quad (18)$$

$$\hat{\Pi}_-^{(i)} = -i \sum_m \hat{a}_{m-1}^{(i)} \hat{a}_m^{(i)\dagger}, \quad (19)$$

$$\hat{\Pi}_3^{(i)} = \sum_m \hat{N}_m^{(i)}. \quad (20)$$

Another important quantity is the angular momentum

$$\mathbf{J} = \frac{1}{4\pi c} \int_{\mathcal{V}} \mathbf{r} \times [\mathbf{E}(\mathbf{r}, t) \times \mathbf{B}(\mathbf{r}, t)] dV. \quad (21)$$

Taking \mathcal{V} as the whole space, using the standard decomposition,

$$\begin{aligned} \mathbf{J} = & \frac{1}{4\pi c} \int_{\mathcal{V}} E_i [\mathbf{r} \times \nabla] A_i dV + \frac{1}{4\pi c} \int_{\mathcal{V}} \mathbf{E} \times \mathbf{A} dV \\ & - \frac{1}{4\pi c} \oint_S \mathbf{E} [\mathbf{r} \times \mathbf{A}] \cdot d\mathbf{s}, \end{aligned} \quad (22)$$

the expression

$$\hat{L}_z = \frac{1}{4\pi c} \int_{\mathcal{V}} \hat{E}_i [\mathbf{r} \times \nabla]_z \hat{A}_i dV = \hbar \sum_{i,m} \int dk_{\perp} dk_z m \hat{N}_m^{(i)} \quad (23)$$

follows for the orbital angular momentum along the z axis and

$$\begin{aligned} \hat{W}_z = & \frac{1}{4\pi c} \int_{\mathcal{V}} (\mathbf{E} \times \mathbf{A})_z dV \\ = & \hbar \sum_m \int dk_{\perp} dk_z \frac{c}{2\omega} ik_z (\hat{a}_m^{(\text{TM})\dagger} \hat{a}_m^{(\text{TE})} - \hat{a}_m^{(\text{TM})} \hat{a}_m^{(\text{TE})\dagger}) \end{aligned} \quad (24)$$

represents the helicity operator. The surface integral in Eq. (22) is not well defined for the elementary TE and TM modes because they do not decay rapidly enough as $r \rightarrow \infty$. Similar but not identical expressions for \hat{L}_z and \hat{W}_z are reported in Ref. [6]. The differences are apparently due to additional boundary conditions imposed in [6] at surfaces with $\rho = \text{constant}$.

The Hamiltonian describing the system formed by the atom and the electromagnetic radiation is taken to be

$$\hat{H} = \hat{H}_p + \hat{H}_R + \hat{H}_I, \quad (25)$$

with \hat{H}_I the interaction Hamiltonian. The latter results from minimal coupling of the particles and the electromagnetic field in Coulomb gauge, as well as the magnetic interaction between the magnetic moment $g_i q_i / 2M_i \mathbf{S}_i$ associated to the spin of each particle \mathbf{S}_i with the radiation magnetic field \mathbf{B} ,

$$\hat{H}_I = \hat{H}_{I1} + \hat{H}_{I2} + \hat{H}_{I3}, \quad (26)$$

$$\hat{H}_{I1} = - \sum_{i=1}^2 \frac{q_i}{M_i} \mathbf{p}_i \cdot \hat{\mathbf{A}}(\mathbf{r}_i), \quad (27)$$

$$\hat{H}_{I2} = \sum_{i=1}^2 \frac{q_i^2}{2M_i} |\hat{\mathbf{A}}(\mathbf{r}_i)|^2, \quad (28)$$

$$\hat{H}_{I3} = - \sum_{i=1}^2 g_i \frac{q_i}{2M_i} \mathbf{S}_i \cdot \hat{\mathbf{B}}(\mathbf{r}_i). \quad (29)$$

III. MATRIX ELEMENTS OF THE INTERACTION HAMILTONIAN

A. The interaction Hamiltonian H_{I1}

The first order perturbation theory probability amplitude of emission of a Bessel photon $\mathbf{A}_{\kappa}^{(i)}$ when the atom makes a transition between an initial Ψ_0 and a final state Ψ_F via the interaction Hamiltonian H_{I1} can be written as

$$\begin{aligned} \langle F, 1_{\kappa}^{(i)} | H_{I1} | 0; 0 \rangle = & \frac{1}{i\hbar} (E_{CM}^{(0)} - E_{CM}^{(F)}) \int d^3r d^3R [\Psi_F^*(\mathbf{r}, \mathbf{R}) \mathbf{R} \Psi_0^*(\mathbf{r}, \mathbf{R})] \left[q_e \mathbf{A}_{\kappa}^{(i)*} \left(\mathbf{R} + \frac{\mu}{M_e} \mathbf{r} \right) + q_N \mathbf{A}_{\kappa}^{(i)*} \left(\mathbf{R} - \frac{\mu}{M_N} \mathbf{r} \right) \right] + \frac{1}{i\hbar} (E_{\text{rel}}^{(0)} \\ & - E_{\text{rel}}^{(F)}) \int d^3r d^3R [\Psi_F^*(\mathbf{r}, \mathbf{R}) \mathbf{r} \Psi_0^*(\mathbf{r}, \mathbf{R})] \left[q_e \frac{\mu}{M_e} \mathbf{A}_{\kappa}^{(i)*} \left(\mathbf{R} + \frac{\mu}{M_e} \mathbf{r} \right) - q_N \frac{\mu}{M_N} \mathbf{A}_{\kappa}^{(i)*} \left(\mathbf{R} - \frac{\mu}{M_N} \mathbf{r} \right) \right] \end{aligned} \quad (30)$$

as long as the separability conditions (5) are satisfied.

Let us define

$$\xi_{lm}(\rho, \varphi; k_{\perp}) = J_l(k_{\perp} \rho) e^{im\varphi} \quad (31)$$

and consider the case where the argument of the Bessel function refers to a transverse vector $\tilde{\rho}$ that can be written as the vector sum of two transverse vectors $\tilde{\rho} = \mathbf{R}_{\perp} - \mathbf{q}_{\perp}$. For $l > 0$ the Gegenbauer sum rule [16] establishes that

$$\begin{aligned} \frac{J_l(k_{\perp} \rho)}{(k_{\perp} \rho)^l} = & 2^l (l-1)! \sum_{v=0}^{\infty} (l \\ & + v) \frac{J_{l+v}(k_{\perp} R_{\perp}) J_{l+v}(k_{\perp} q_{\perp})}{(k_{\perp} R_{\perp})^l (k_{\perp} q_{\perp})^l} C_v^l [\cos(\varphi_R - \varphi_q)], \end{aligned}$$

$$C_v^l = \sum_{s=0}^v \frac{\Gamma(l+s) \Gamma(l+v-s)}{s! (v-s)! [\Gamma(l)]^2} \cos[(v-2s)(\varphi_R - \varphi_q)], \quad (32)$$

while it can be shown that [8]

$$e^{im\varphi} = \sum_{n=0}^m (-1)^n \binom{m}{n} e^{i(m-n)\varphi_R} e^{in\varphi_q} \left(\frac{(k_{\perp} R_{\perp})^{m-n} (k_{\perp} q_{\perp})^n}{(k_{\perp} \rho)^m} \right). \quad (33)$$

Thus, for $m > 0$,

$$\begin{aligned} \psi_m(\rho, \varphi; k_\perp) = \xi_{mm}(\rho, \varphi; k_\perp) = 2^m(m-1)! \sum_{v=0}^{\infty} (m+v) \frac{J_{m+v}(k_\perp R_\perp) J_{m+v}(k_\perp q_\perp)}{(k_\perp q_\perp)^m} \sum_{s=0}^v \frac{\Gamma(m+s)\Gamma(m+v-s)}{s!(v-s)!(\Gamma(m))^2} \cos[(v-2s)(\varphi_R \\ - \varphi_q)] \sum_{n=0}^m (-1)^n \binom{m}{n} \left(\frac{q_\perp}{R_\perp}\right)^n e^{i(m-n)\varphi_R} e^{in\varphi_q}, \end{aligned} \quad (34)$$

while, for $m=0$ [16],

$$\psi_0(\rho, \varphi; k_\perp) = J_0(k_\perp \rho) = \sum_{v=-\infty}^{\infty} J_v(k_\perp R_\perp) J_v(k_\perp q_\perp) \cos[v(\varphi_R - \varphi_q)]. \quad (35)$$

These equations are the basis of the multipolar expansion of the transition amplitude (30) in cylindrical coordinates. The relevant values of the vector \mathbf{q} are $\mathbf{q}=(\mu/M_e)\mathbf{r}$ and $\mathbf{q}=- (\mu/M_N)\mathbf{r}$. Before performing explicit multipole calculations, we show an important result for the emission of a Bessel photon valid when the center of mass and relative wave functions are of the form

$$\begin{aligned} \Phi(\mathbf{R}) &= \frac{1}{\sqrt{2\pi}} e^{im_R \varphi_R} Y_{CM}(R_\perp, z_R), \\ \phi(\mathbf{r}) &= \Theta(r) Y_{lm_r}(\theta, \varphi_r), \end{aligned} \quad (36)$$

with Y_{lm} the spherical harmonics. In this case, the integration over the azimuthal angles φ_R and φ_r leads to selection rules related to the conservation of angular momentum in the z direction. A direct examination of Eq. (30) and Eqs. (34) and (35) shows that these selection rules are of the form

$$\begin{aligned} m - n \pm v \mp 2s - m &= m_R - m'_R, \\ n \mp v \pm 2s &= m_r - m'_r, \end{aligned} \quad (37)$$

for the transition amplitudes proportional to $E_{CM}^{(0)} - E_{CM}^{(F)}$, and

$$\begin{aligned} m - i - n \pm v \mp 2s &= m_R - m'_R, \\ i + n \mp v \pm 2s &= m_r - m'_r, \end{aligned} \quad (38)$$

with $i=\pm 1, 0$, for the transition amplitudes proportional to $E_{\text{rel}}^{(0)} - E_{\text{rel}}^{(F)}$. Here the letters n , s , and v denote the summation indices as they appear in Eq. (34). The first (second) equality in Eqs. (37) and (38) permits the identification of the angular momentum acquired by the center of mass (internal motion) in the corresponding emission process. These results are consistent with those reported in Refs. [6,7] for the dipole and quadrupole transitions. Notice that the total change in the projection of the angular momentum of the atom along the z axis is always $-m\hbar$. The conservation of angular momentum implies that the total angular momentum of the Bessel photon is $m\hbar$. Thus the helicity term in Eq. (22) obtained from standard quantum optics definitions must be somehow compensated by the surface integral.

Now, consider the cases for which the longitudinal and transverse long wavelength approximations $k_z z_r \ll 1$ and $k_\perp \rho_r \ll 1$ are valid. These conditions are satisfied for optical Bessel beams and standard atomic systems. Notice that $0 \leq n \leq m$ is the index related to a series expansion on powers of q_\perp/R_\perp in Eq. (34), and that due to the relation

$$\frac{J_{m+v}(k_\perp q_\perp)}{(k_\perp q_\perp)^m} = \left(\frac{k_\perp q_\perp}{2}\right)^v \sum_{t=0}^{\infty} (-1)^t \frac{(k_\perp q_\perp)^{2t}}{2^{2t} t! (m+v+t)!}, \quad (39)$$

v can be regarded as an index related to a power expansion useful for a long wavelength approximation. For $k_\perp q_\perp \ll 1$ the term $v=0$ is expected to be dominant in the series expansion of the vector potential and the functions ψ_m can be approximated by

$$\psi_m \sim J_m(k_\perp R_\perp) \sum_{n=0}^m (-1)^n \binom{m}{n} \left(\frac{q_\perp}{R_\perp}\right)^n e^{i(m-n)\varphi_R} e^{in\varphi_q}. \quad (40)$$

If the atom is located outside the axes of the Bessel beam then, in general, $q_\perp \ll R_\perp$ and the $n=0$ term is dominant. Under such conditions the neutral atom ($q_e = -q_N$) transition amplitude

$$\begin{aligned} \langle F, 1_K^{(i)} | H_{I1} | 0; 0 \rangle &\sim \frac{q_e}{i\hbar} (E_{\text{rel}}^0 - E_{\text{rel}}^F) \\ &\times \int d^3R \Phi_0^*(\mathbf{R}) \mathbf{A}_K^{(i)*}(\mathbf{R}) \Phi_F(\mathbf{R}) \\ &\times \int d^3r \phi_F^*(\mathbf{r}) \mathbf{r} \phi_0(\mathbf{r}) \end{aligned} \quad (41)$$

contains the standard dipole matrix element for the relative coordinates. If the center of mass and internal wave functions are given by Eq. (36), the transition amplitude can be written as

$$\begin{aligned} \langle F, 1_K^{\text{TE}} | H_{I1} | 0; 0 \rangle &\sim \frac{q_e E_0}{k_z \hbar} (E_{\text{rel}}^0 - E_{\text{rel}}^F) e^{-i[\omega t - (E_F - E_0)t/\hbar]} \\ &\times \sum_{j=\pm 1} \delta_{m-j, m_R - m'_R} \delta_{j, m'_r - m_r} I_{CM}^{(0)}(k_\perp, k_z, m \\ &- j) I_{\text{rel}}(k_\perp, k_z, j), \end{aligned} \quad (42)$$

while

$$\begin{aligned}
 \langle F, 1_K^{\text{TM}} | H_{I1} | 0; 0 \rangle &\sim \frac{q_e E_0 c}{i \hbar \omega} (E_{\text{rel}}^0 - E_{\text{rel}}^F) e^{-i[\omega t - (E_F - E_0)t/\hbar]} \\
 &\times \left(-\frac{2k_{\perp} i}{k_z} [\delta_{m, m'_R - m_R} \delta_{m'_r, m_r} I_{CM}^{(0)} \right. \\
 &\times (k_{\perp}, k_z, m) I_{\text{rel}}(k_{\perp}, k_z, 0) \\
 &+ \sum_{j=\pm 1} (-j) \delta_{m-j, m_R - m'_R} \delta_{j, m'_r - m_r} I_{CM}^{(0)}(k_{\perp}, k_z, m \\
 &\left. - j) I_{\text{rel}}(k_{\perp}, k_z, j) \right], \quad (43)
 \end{aligned}$$

with

$$\begin{aligned}
 I_{CM}^{(0)}(k_{\perp}, k_z, m-j) &= \int dR_{\perp} dz Y_{CM}^{F*}(R_{\perp}, z) e^{ik_z z} J_{m-j}(k_{\perp} R_{\perp}) \\
 &\times Y_{CM}^0(R_{\perp}, z) \quad (44)
 \end{aligned}$$

and

$$\begin{aligned}
 I_{\text{rel}}(k_{\perp}, k_z, j) &= \frac{1}{2l'_r + 1} \left\{ \delta_{j,0} [(l'_r - |m_r| + 1) \delta_{l'_r, l'_r + 1} + (l'_r - |m_r| \right. \\
 &- 1)] + (1 - \delta_{j,0}) [\delta_{l'_r, l'_r + 1} \delta_{|m_r|, |m'_r| - 1} \\
 &\left. - \delta_{l'_r, l'_r - 1} \delta_{|m_r|, |m'_r| + 1}] \right\} \int dr r^3 \Theta_F^*(r) \Theta_0(r). \quad (45)
 \end{aligned}$$

$$\begin{aligned}
 \left[\frac{\mu}{M_e} \xi_{mm} \left(\mathbf{R} + \frac{\mu}{M_e} \mathbf{r} \right) - \frac{\mu}{M_N} \xi_{mm} \left(\mathbf{R} - \frac{\mu}{M_N} \mathbf{r} \right) \right] &\sim e^{im\varphi_R} J_m(k_{\perp} R_{\perp}) + \left(\frac{\mu}{M_e} \right)^2 k_{\perp} r_{\perp} J_{m+1}(k_{\perp} R_{\perp}) \cos(\varphi_R - \varphi_r) e^{im\varphi_R} \\
 &+ (1 - \delta_{m,0}) \frac{\mu}{M_e} \left[\sum_{n=1}^m \binom{m}{n} \left(\frac{r_{\perp}}{R_{\perp}} \right)^n e^{i(m-n)\varphi_R} e^{in\varphi_r} \right] \left(J_m(k_{\perp} R_{\perp}) \right. \\
 &\left. + \frac{\mu}{M_e} J_{m+1}(k_{\perp} R_{\perp}) k_{\perp} r_{\perp} \cos(\varphi_R - \varphi_r) \right), \quad (46)
 \end{aligned}$$

and at the same order in $k_z q_z$,

$$e^{ik_z(z_R + q_z)} \sim e^{ik_z z_R} (1 + ik_z q_z). \quad (47)$$

When inserted in the transition probability amplitude, Eq. (30), the terms proportional to r_{\perp} and z in the last two equations lead to matrix elements of the relative motion of the quadrupole type $x_i x_j$. As a consequence, standard selection rules are obtained for that degree of freedom, e. g., $\Delta m_z^{\text{rel}} = \pm 2\hbar, \pm 1\hbar, 0$.

The terms in Eq. (46) with $n > 0$ are expected to be relevant only when the atomic center of mass is located close to the axis of symmetry of the Bessel mode. However, there is a vortex of charge m at that axis and $J_m(k_{\perp} \rho) = 0$ for $\rho = 0$ if $m \neq 0$. Thus, even if the center of mass is properly located, the matrix element is expected to be small. To explicitly

As expected, the selection rules for transitions involving the relative motion of the charged particles are the same as those obtained with a plane wave expansion of the radiation potential. Notice, however, that according to Eqs. (42) and (43), the emission of a Bessel photon of orbital angular momentum $m\hbar$ yielding $m'_r = m_r \pm 1$ leads to a rotational recoil effect $m'_R = m_R - m \mp 1$ for the center of mass while, to this order of approximation, transitions with $m'_r = m_r$ and $m'_R = m_R - m$ are allowed just for the emission of transverse magnetic photons. These transitions favor torque effects on the center of mass and are specially relevant in the emission of nonparaxial photons. The idea that rotational recoil effects on the center of mass motion could occur for Bessel photons can be traced out to the work of van Enk and Nienhuis [6,7]

Going beyond the approximation corresponding to Eq. (41) requires to consider both terms with $n > 0$ in the series (40) and terms with $v > 0$ in Eqs. (34) and (35). In the case of atoms with $M_N \gg M_e$, the energy involved in changes of the center of mass motion is usually several orders of magnitude smaller than the energy involved in changes of the internal state. As a consequence, the important terms are those proportional to $E_{\text{rel}}^{(0)} - E_{\text{rel}}^{(F)}$ in Eq. (30); for them, to lowest order in μ/M_N and first order in $k_{\perp} r_{\perp}$,

quantify this effect, consider two specific situations. In the first, the center of mass states correspond to a free atom

$$Y_{CM}^{\text{Free}}(R_{\perp}, z_R) = N_{CM} J_{m_R}(k_{\perp} R_{\perp}) e^{ik_z^R z_R}. \quad (48)$$

In the second, the atom is trapped by an external harmonic potential

$$Y_{CM}^{\text{HO}}(R_{\perp}, z_R) = N_{CM} e^{-R_{\perp}^2/2\alpha^2} \left(\frac{R_{\perp}}{\alpha} \right)^{|m_R|} L_{\bar{n}}^{|m_R|} (R_{\perp}^2/\alpha^2) e^{ik_z^R z_R}. \quad (49)$$

Here $\bar{n} = (N_R - m_R)/2$, and N_R is the quantum number giving the energy of the oscillator $E_R = \hbar \Omega_R (N_R + 1)$, Ω_R is the frequency of the oscillator and $\alpha = \sqrt{\hbar/M_N \Omega_R}$ is the natural amplitude of the oscillator.

For simplicity, in both the free and trapped atom cases, we take the symmetry axis of the center of mass motion to coincide with the axis of the Bessel mode. According to Ref. [17], if

$$\begin{aligned} \mathcal{I}(k_{\perp}, k_{\perp}^R, k_{\perp}^{R'}, m, n) = & \int_0^{\infty} J_m(k_{\perp} R_{\perp}) R_{\perp}^{-n+1} \\ & \times J_{m_R}(k_{\perp}^R R_{\perp}) J_{m_{R'}+m-n}(k_{\perp}^{R'} R_{\perp}) \end{aligned} \quad (50)$$

then

$$\mathcal{I}(k_{\perp}, k_{\perp}^R, k_{\perp}^{R'}, m, n) = 0, \quad (51)$$

whenever $k_{\perp}^{R'} > k_{\perp} + k_{\perp}^R$, while

$$\begin{aligned} \mathcal{I}(k_{\perp}, k_{\perp}^R, k_{\perp}^{R'}, m, n) = & 2^{-n+2} k_{\perp}^m (k_{\perp}^R)^{m_R} (k_{\perp}^{R'})^{m+m_R-2} \\ & \times \frac{\Gamma[3(m_R + m - n)/2 + 2]}{m! m_R!} \\ & \times \sum_{u,v=0}^{\infty} \frac{(m_R + m - n + 1)_{u+v}}{(1+m)_u (1+m_R)_v u! v!} \\ & \times \left(\frac{k_{\perp}}{k_{\perp}^{R'}} \right)^{2u} \left(\frac{k_{\perp}^R}{k_{\perp}^{R'}} \right)^{2v} \end{aligned} \quad (52)$$

otherwise.

Equation (51) reflects the conservation of transverse momentum, and Eq. (52) shows that the transition amplitude for $n > 0$ decreases as n increases (each coefficient in the series expansion of positive terms decreases as n increases). Notice also that a free center of mass wave function is normalized in terms of delta distributions. For free atoms, a comparison with experimental results would require working with wave packets.

For an atom trapped in a harmonic potential, a direct use of the integral

$$\begin{aligned} & \int_0^{\infty} dx x^{\nu+1} e^{-x^2/\alpha^2} L_{\lambda}^{\nu-\sigma}(x^2/\alpha^2) L_{\eta}^{\sigma}(x^2/\alpha^2) J_{\nu}(kx) \\ & = (-1)^{\lambda+\eta} (2/\sqrt{\alpha})^{-\nu-1} k^{\nu} e^{-(\alpha^2 k^2/4)} L_{\eta}^{\sigma-\lambda-\eta}(\alpha^2 k^2/4) \\ & \quad \times L_{\lambda}^{\nu-\sigma+\lambda-\eta}(\alpha^2 k^2/4) \end{aligned} \quad (53)$$

shows that even for $n=0$ the transition amplitude depends exponentially on the ratio of the spread of the harmonic wave function and the transversal wavelength $k_{\perp}^2 \alpha^2$. The case $n > 0$ can be treated analytically if the center of mass initial wave function corresponds to the ground state oscillations ($N=0$ and $m_R=0$). In that case, we can use the expression [18]

$$\begin{aligned} & \int_0^{\infty} dx x^{\nu-1} J_{\mu}(b\sqrt{x}) L_n^{\lambda}(cx) e^{-cx} \\ & = \frac{b^{\mu} (1-\nu-\mu+\lambda)_n \Gamma(\nu+\mu/2)}{2^{\mu} n! c^{\nu+\mu/2} \Gamma(\mu+1)} \\ & \quad \times {}_2F_2\left(\nu+\mu/2, \nu+\mu/2-\lambda; \nu+\mu/2-\lambda-n, \mu+1; -\frac{b^2}{4c}\right) \end{aligned} \quad (54)$$

to show that

$$\begin{aligned} & \mathcal{J}(\bar{n}, \alpha, k_{\perp}, m) \\ & = (\sqrt{\alpha})^{n-m} \int_0^{\infty} R_{\perp}^{m-2n+1} e^{\rho_{\perp}^2/\alpha^2} J_m(k_{\perp} R_{\perp}) L_{\bar{n}}^{m-n}(R_{\perp}^2/\alpha^2) \\ & = \frac{k_{\perp}^{m+2n}}{2^{m+2n+1} \bar{n}! (\sqrt{\alpha})^{-\bar{n}-1}} \sum_{r=0}^{\infty} \frac{(m+\bar{n}-n+r)!}{(m+\bar{n}+r)! r!} \\ & \quad \times \left(\frac{-k_{\perp}^2 \alpha^2}{4} \right)^r. \end{aligned} \quad (55)$$

Notice that the terms of this series with $r \gg n$ behave as the exponential series terms, so that series (55) is convergent even if $k_{\perp}^2 \alpha^2/4 > 1$.

B. Matrix elements of the interaction term H_{I2}

The lowest order contribution of the interaction \hat{H}_{I2} to spontaneous emission of light from vacuum is quadratic in the coupling constant q_i and, to this order, involves necessarily two photons. For a hydrogenic atom, the value of the electron-proton mass ratio implies that $q_e^2/2M_e \gg q_N^2/2M_N$ and also

$$\hat{H}_{I2} \sim \frac{q_e^2}{2M_e} \left| \hat{\mathbf{A}} \left(\mathbf{R} + \frac{\mu}{M_e} \mathbf{r} \right) \right|^2. \quad (56)$$

In the long wavelength limit, one can use the approximation to the products

$$\begin{aligned} & \psi_m \left(\mathbf{R}_{\perp} + \frac{\mu}{M_e} \mathbf{r}_{\perp}, z \right) \psi_{m'} \left(\mathbf{R}_{\perp} + \frac{\mu}{M_e} \mathbf{r}_{\perp}, z \right) \\ & \sim e^{i(k_z+k'_z)z} e^{-i(\omega+\omega')t} J_m(k_{\perp} R_{\perp}) \end{aligned} \quad (57)$$

$$\begin{aligned} & \times J_{m'}(k'_{\perp} R_{\perp}) \sum_{n,n'=0}^m \binom{m}{n} \binom{m'}{n'} \\ & \times \left(-\frac{\mu}{M_e} \frac{r_{\perp}}{R_{\perp}} \right)^{(n+n')} e^{i(m+m'-n-n')\varphi_R} e^{i(n+n')\varphi_r} \end{aligned} \quad (58)$$

in the expression for the relevant electromagnetic modes. As a consequence, unless the atom is located on the beam axis, it should be expected that the most important contributions to the transition probabilities come from the $n=n'=0$ terms in these series. The two photons are then emitted producing a

translational and rotational recoil effect on the center of mass, while the internal state of the atom remains invariant. Higher order effects can be directly calculated using Eqs. (34) and (35).

C. Matrix elements of the interaction term H_{I3}

The interaction term \hat{H}_{I3} makes it possible to change the spin of the particles. The corresponding matrix elements can be easily calculated within first order perturbation theory using the identities

$$g_i \frac{q_i}{2M_i} \mathbf{S}_i \cdot \hat{\mathbf{B}}^{(\text{TM})}(\mathbf{r}_i) = g_i \frac{q_i \omega}{4M_i c k_z} E_0 [\psi_{m-1}(\mathbf{r}_i) \hat{S}_+^{(i)} + \psi_{m+1}(\mathbf{r}_i) \hat{S}_-^{(i)}], \quad (59)$$

$$g_i \frac{q_i}{2M_i} \mathbf{S}_i \cdot \hat{\mathbf{B}}^{(\text{TE})}(\mathbf{r}_i) = g_i \frac{iq_i}{4M_i} E_0 \left(\psi_{m-1}(\mathbf{r}_i) \hat{S}_+^{(i)} - \psi_{m+1}(\mathbf{r}_i) \hat{S}_-^{(i)} - \frac{2ik_\perp}{k_z} \psi_m(\mathbf{r}_i) \hat{S}_z^{(i)} \right), \quad (60)$$

with S_\pm the ascending and descending spin operators. Again, Eqs. (34) and (35) lead to a multipole expansion for the matrix elements. For hydrogenic atoms, the ratio q_i/M_i is larger for electrons than for nuclei, so that the most probable event of this type produces changes of the spin angular momentum of the electron by a factor $\pm\hbar$ without changing the spatial wave function of relative motion, while the center of mass acquires an angular momentum $-(m \mp 1)\hbar$. The event corresponding to no changes in the internal wave function at the expense of a recoil effect with a change of the orbital angular momentum of the center of mass by $-m\hbar$ is also relevant for nonparaxial photons. Notice that the matrix elements calculated for H_{I1} with the proper identifications are useful in the evaluation of the transition amplitudes associated to H_{I3} .

IV. COMPARISON WITH SOME PREVIOUS RESULTS IN THE PARAXIAL APPROXIMATION

Now let us compare our results to those obtained by Babiker *et al.* [8] who studied the transition amplitude for the emission of electromagnetic photons of the generic type

$$\mathbf{A}(\mathbf{x}, t) = \hat{\mathbf{e}}F(x_\perp) e^{i(k_z x_z - \omega t)} e^{im\varphi} \quad (61)$$

by hydrogenic atoms within the PZW formalism [19,20]. The fields (61) can be considered a paraxial approximation to the so-called left and right polarized Bessel modes [9,21],

$$\mathbf{A}_m^{(\mathcal{L})}(\mathbf{x}, t; k_\perp, k_z) = A_0^{(\mathcal{L})} \left[(\mathbf{e}_x + i\mathbf{e}_y) \psi_m - i \left(\frac{k_\perp}{k_z} \right) \psi_{m+1} \mathbf{e}_z \right], \quad (62)$$

$$\mathbf{A}_m^{(\mathcal{R})}(\mathbf{x}, t; k_\perp, k_z) = A_0^{(\mathcal{R})} \left[(\mathbf{e}_x - i\mathbf{e}_y) \psi_m + i \left(\frac{k_\perp}{k_z} \right) \psi_{m-1} \mathbf{e}_z \right]. \quad (63)$$

Their superpositions $\mathbf{A}_m^{(\mathcal{R})} \pm \mathbf{A}_m^{(\mathcal{L})}$ define linearly polarized modes, and are linear combinations of the elementary TE and TM modes,

$$\mathbf{A}_m^{(\mathcal{L})} = A_0^{(\mathcal{L})} \left(\mathbf{A}_{m+1}^{(\text{TM})} - i \frac{ck_z}{\omega} \mathbf{A}_{m+1}^{(\text{TE})} \right), \quad (64)$$

$$\mathbf{A}_m^{(\mathcal{R})} = A_0^{(\mathcal{R})} \left(\mathbf{A}_{m-1}^{(\text{TM})} + i \frac{ck_z}{\omega} \mathbf{A}_{m-1}^{(\text{TE})} \right). \quad (65)$$

Notice that an index m for the polarized modes corresponds to the superposition of TE and TM modes with $m \pm 1$. According to the results we have obtained, the corresponding left and right polarized Bessel beams carry an angular momentum $(m \pm 1)\hbar$ along the z axis.

In the present work we have an explicit form for the generic function $F(x_\perp)$ and we obtained a complete multipole expansion that takes into account both the azimuthal and radial behavior of electromagnetic Bessel modes. Accordingly, these transition amplitudes extend the results of Babiker *et al.* beyond the paraxial limit. Using Eqs. (64) and (65), it is straightforward to show that our results are consistent with those reported in Ref. [8]. However, there are some conceptual differences between both approaches. The total angular momentum for TE and TM photons is $m\hbar$ and cannot be directly separated into orbital or spin parts. For the superpositions of the TE and TM modes leading to \mathcal{L} and \mathcal{R} modes, this separation seems more natural and permitted Babiker *et al.* to conclude that “in the interaction of molecules with light endowed with **orbital** angular momentum, an exchange of **orbital** angular momentum in an electric dipole transition occurs only between the light and the center of mass motion.”

Nevertheless, the circularly polarized modes \mathcal{R} and \mathcal{L} do not form an orthogonal basis. This has consequences when performing a quantization of the electromagnetic field in terms of them. By choosing $A_0^{(\mathcal{L})} = A_0^{(\mathcal{R})} = \sqrt{1 + c^2 k_z^2 / \omega^2} / 2$ the corresponding creation and annihilation operators satisfy the standard commutation relations

$$[\hat{a}_m^{(\mathcal{L})}(k_z, k_\perp), \hat{a}_{m'}^{(\mathcal{L})\dagger}(k'_z, k'_\perp)] = \frac{1}{k_\perp} \delta_{m,m'} \delta(k_\perp - k'_\perp) \delta(k_z - k'_z),$$

$$[\hat{a}_m^{(\mathcal{R})}(k_z, k_\perp), \hat{a}_{m'}^{(\mathcal{R})\dagger}(k'_z, k'_\perp)] = \frac{1}{k_\perp} \delta_{m,m'} \delta(k_\perp - k'_\perp) \delta(k_z - k'_z). \quad (66)$$

However, not all the other commutators are zero, in fact

$$[\hat{a}_m^{(\mathcal{L})}(k_z, k_\perp), \hat{a}_{m'+2}^{(\mathcal{R})\dagger}(k'_z, k'_\perp)] = \frac{1 - c^2 k_z^2 / \omega^2}{1 + c^2 k_z^2 / \omega^2} \frac{1}{k_\perp} \delta_{m,m'} \delta(k_\perp - k'_\perp) \delta(k_z - k'_z). \quad (67)$$

These results make it more difficult to interpret the dynamical observables of the field written in terms of creation and

annihilation operators. For instance, the energy is not diagonal in this basis [15].

Thus, the idea that internal angular momentum of the atom and the spin of the photon as well as the center of mass angular momentum and the orbital angular momentum of the photon are separately conserved is just valid in the paraxial approximation [6]. Besides, when the identification of circularly polarized Bessel photons is made with the modes (64) and (65) care must be taken because they are not an orthogonal set. An alternative in this case is to consider the superpositions $\mathbf{A}^{(\pm)} = A_0^\pm (\mathbf{A}^{\text{TM}\pm} + \mathbf{A}^{\text{TE}})$ which diagonalize W_z given by Eq. (24) and constitute an orthonormal set [15].

V. CONCLUSIONS AND DISCUSSION

In this Paper we have calculated the emission probability amplitude of a Bessel photon by an atomic system within first order perturbation theory. We obtained a closed expression of the electromagnetic potentials that permits a systematic multipole approximation taking into account both the azimuthal and radial behavior of the electromagnetic Bessel modes.

It was shown that the emission of a Bessel TE or TM photon of order m induces a change in the projection of angular momentum along the z axis of the atom that is always of magnitude $\hbar m$. Thus, the angular momentum carried by these Bessel photons is precisely $\hbar m$. Similar results were obtained by van Enk and Nienhuis [6,7]. Nevertheless, their relevance must be emphasized because a field theoretical description of the angular momentum of the electromagnetic field in terms of TE and TM Bessel modes leads to Eq. (22). The second term in this equation is usually related to spin angular momentum, while the surface integral is not well defined. Thus, the calculations here performed show the relevance of the surface terms and are a direct dynamical evaluation of the total angular momentum z component of a Bessel photon.

It is important to notice, as van Enk and Nienhuis did [6], that the vectorial character of the electromagnetic field is responsible for possible changes $\pm\hbar$ in the internal angular momentum within the dipole approximation. As usual, these changes are induced by the field components along the circular vectors $\hat{\mathbf{e}}_x \pm \hat{\mathbf{e}}_y$. The corresponding transition probabilities are proportional to $E_0^2 \sim k_z^2 k_\perp^2 / \omega$ as can be seen from Eq. (11). The transition probability of emission of TM Bessel photons via H_{I1} without changes in the internal angular momentum necessarily leads to the maximum possible exchange of angular momentum between a Bessel photon and the center of mass motion. These transition probabilities are proportional to $E_0^2 k_\perp^2 / k_z^2 \sim k_\perp^3 c^2 / \omega$ and they could be important for nonparaxial Bessel photons.

The fact that spontaneously emitted optical Bessel photons have not been observed can be due to the small value of the center of mass matrix elements under usual circumstances. In this paper, we have explicitly evaluated these elements both for free atoms and for harmonically trapped atoms. In the first case, the conservation of linear momentum in the radial direction do not single out a particular value of

$k_\perp^{R'}$; this is an important difference with the result obtained in the axial direction for which the matrix element is proportional to $\delta(k_z^{R'} - k_z^R + k_z)$. Notice that both the radial and axial photon functions are normalized via delta distributions; that is, the matrix elements for the emission of a photon with specific k_\perp , starting from a specified wave function of the center of mass with a given k_\perp^R , are finite and different from zero for a continuum range of values of the final transversal momentum for the center of mass $k_\perp^{R'}$. As a consequence, the idealized case of a transition between initial and final states for the center of mass represented by Bessel functions, has an effectively zero probability. In any case, comparison with experimental results would require working with wave packets. For trapped atoms, the transverse part of the center of mass wave function is localized. The transition amplitude depends on the average position of the center of mass and on the spread of the oscillation α . We have shown that the matrix element of the center of mass motion given by the standard electric dipole matrix for the internal motion, Eq. (41), is proportional to two factors. The first is the coefficient $k_\perp^{m+2n} / \alpha^{n/2}$ and the second decays exponentially with the factor $k_\perp^2 \alpha^2 / 4$ relating the spread of the atom oscillation to the photon wavelength. For paraxial beams and highly localized trapped atoms, the condition $k_\perp^2 \alpha^2 \ll 1$ is currently feasible. Simultaneously, to observe this effect the atom localization must be such that $k_\perp^{m+2n} / \alpha^{n/2}$ is not too small.

We have focused our attention on spontaneous transition amplitudes, but induced transition probabilities can also be calculated from them using Einstein relations. They will be proportional to incident radiation intensity and could experimentally confirm our results. We have explicitly shown that certain mechanisms can enhance the probability of changing the internal angular momentum of the atom in multiples of \hbar larger than those predicted by the standard plane wave multipole expansion. For instance, transitions with $\Delta m' = \pm 2\hbar$ depend on the electric quadrupole matrix elements of the relative motion and are given by two kinds of transition amplitudes: one for the standard quadrupole expansion that is proportional to k_\perp and the other arising from terms with $n = 1$ and $k = 0$ in Eq. (34). The latter are due to the vortex of the Bessel mode in the beam axes and could be detected for a trapped atom with an adequate value of k_\perp and α , Eq. (58).

Finally, we have analyzed some specific features of the transition amplitudes associated to the interaction Hamiltonian H_{I2} and H_{I3} . In the long wavelength limit, the most important transitions associated to the former Hamiltonian involve two photons that do not alter the internal motion of the atom but exchange linear, $\hbar(k_z + k_z')$, and angular momentum, $(m + m')\hbar$, with the center of mass. For hydrogenic atoms, the magnetic interaction $g_i q_i / 2M_i \mathbf{S}_i \cdot \hat{\mathbf{B}}(\mathbf{r}_i)$ will favor changes in the spin orientation of the electron $\pm\hbar$ and in the orbital angular momentum of the center of mass.

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