Formulation of the twisted-light–matter interaction at the phase singularity: the twisted-light gauge

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Twisted light is light carrying orbital angular momentum. The profile of such a beam is a ring-like structure with a node at the beam axis, where a phase singularity exits. Due to the strong spatial inhomogeneity the mathematical description of twisted-light–matter interaction is non-trivial, in particular at the phase singularity, where the commonly used dipole-moment approximation cannot be applied. In this paper we show theoretically that, if the polarization and the orbital angular momentum of the twisted light beam have the same sign, a Hamiltonian similar to the dipole-moment approximation can be derived. However, if the signs of polarization and orbital angular momentum differ, the magnetic parts of the light beam become of significant importance and an interaction Hamiltonian which only accounts for electric fields, as in the dipole moment approximation, is inappropriate. We discuss the consequences of these findings for twisted light excitation of semiconductor nanostructures, e. g. a quantum dot, placed at the phase singularity; nevertheless, our results are equally applicable to the interaction of twisted light with atoms and molecules.

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I. INTRODUCTION

In recent years, there has been intense research work in the topic of highly inhomogeneous light beams, and in particular, in light carrying orbital angular momentum (OAM)–sometimes called twisted light (TL)$^{[1–3]}$. The research in TL spans several areas, such as the generation of beams$^{[4–6]}$, the interaction of TL with atoms and molecules$^{[7–19]}$ or with condensed matter$^{[17,19]}$. TL has already proved to be useful in applications. The most notable example is perhaps the optical trapping and manipulation of microscopic particle$^{[21,22]}$. Applications in other fields are also sought, for example in quantum information technology, where the OAM adds a new degree of freedom encoding more information$^{[23,24]}$. In addition, theoretical studies in solid state physics predict, for instance, that TL can induce electric currents in quantum rings$^{[18]}$, and new electronic transitions (forbidden for plane waves) in quantum dots$^{[17]}$. This all suggests that TL can be a new powerful tool to control quantum states in nanotechnological applications.

Two features of TL are particularly striking. First, TL exhibits a vortex or phase singularity at the beam axis. Second, polarization and OAM are so intermixed that two beams having the same OAM but opposite polarization behave in a completely different way. This is in contrast to what happens to plane waves, where the polarization alone does not determine other important properties. These two features can also be found in other inhomogeneous beams, namely the so-called azimuthally polarized$^{[24,26]}$ fields.

The interaction between TL and matter is particularly interesting due to the inhomogeneous nature of the TL, and it is worth revisiting its mathematical formulation. The most general form to describe the light-matter interaction is the minimal coupling Hamiltonian, where the electromagnetic fields (EM) enter through their potentials. In many cases of interest, the Hamiltonian can be rewritten in terms of EM fields using gauge transformations, i.e. transformations among potentials that preserve the EM fields$^{[27,28]}$. Usually, the transformations are accompanied by approximations. One of the best-known among these Hamiltonians is the dipole-moment approximation (DMA). It can be derived under the assumption that the EM fields vary little in the region where the matter excitation takes place, and effectively is the electric field $E(t)$ treated as spatially homogeneous. The DMA Hamiltonian then takes the form $H = -qr \cdot E(t)$, where $qr = d$ is the dipole moment of the material system. This form of light-matter coupling is advantageous for several reasons: Because the DMA only contains the electric field, it is gauge invariant. In contrast to the minimal coupling Hamiltonian, the momentum operator has a clear physical meaning. Furthermore, due to its structure the light-matter interaction can be easily treated as a perturbation. For sufficiently homogeneous light fields the DMA is perfectly applicable for example in atomic physics and nanoscale systems such as quantum dots, where matter states are highly localized.

When the inhomogeneous nature of the field becomes important the DMA cannot be used. One could perform calculations with the minimal coupling Hamiltonian, which contains the vector potential. Still, it is appealing to work with a Hamiltonian which contains the electric and magnetic fields only, because then the
theory is manifestly gauge invariant. Of course, using the so-called Poincare gauge \cite{28, 29} one can formally rewrite the Hamiltonian in terms of fields, however, it is not always possible to express the fields explicitly. A desirable expression would be one resembling the electric dipole-moment Hamiltonian, but retaining the spatial dependence: \( H = -\mathbf{q} \cdot \mathbf{E}(\mathbf{r}, t) \). We will call this Electric Field Coupling (EFC) Hamiltonian. In addition to the dipole-moment coupling, the EFC Hamiltonian also contains higher order couplings in the electric field, e.g., quadrupole moments.

In some situations the spatial inhomogeneity of the intensity of the field can be kept in a EFC Hamiltonian in a parametric way, while the transition matrix elements are determined by the coupling via the electric dipole term only \cite{30, 34}, which has been used to describe for instance four-wave-mixing phenomena \cite{32, 37}. Because for TL new transitions are induced by its OAM \cite{31}, such an approach would not describe the main feature of TL and, thus, it is crucial to include the spatial dependence also in the transition matrix elements. Under certain assumptions, e.g., for the interaction at the beam maximum, it is possible to cast the Hamiltonian in a EFC form, and thus, describe the modified selection rules \cite{38, 39} for example using a Power-Zienau-Wooley transformation. \cite{40} However, in this paper we show that for TL-matter interaction in the vicinity of the beam axis an EFC Hamiltonian cannot in general be used. This is directly related to the phase singularity and the intermixing of OAM and polarization.

The TL-matter interaction at the phase singularity for highly focused beams has been analyzed using a multipolar expansion for electric and magnetic fields \cite{26, 41}, which already revealed that higher order electric and magnetic terms can be of significant importance. Nevertheless, for a subgroup of TL beams we show that it is possible to derive an electric multipolar Hamiltonian for the TL-matter interaction close to the phase singularity, which offers the advantages of a DMA Hamiltonian.

We organize the article as follows. First we revisit in Sec. II the concepts of gauge transformation, DMA and EFC Hamiltonian necessary to understand the discussion ahead. Next, in Sec. III we introduce the mathematical representations of TL. In Sec. IV using an heuristic derivation much alike the one found in the literature for the DMA, we arrive at the new expression for the TL-matter Hamiltonian. Section V shows that the atypical behavior of the electric and magnetic field of TL is in part responsible for the need to modify the Hamiltonian. Section VI is devoted to a careful derivation of the new Hamiltonian, motivated by the Poincare gauge. We wrap up with the conclusions in Sec. VII.

II. LIGHT - MATTER INTERACTION REVISITED

The starting point for a mathematical description of the effect of light on matter is the minimal coupling Hamiltonian, that expresses the external EM fields in terms of a scalar \( U(\mathbf{r}, t) \) and a vector \( \mathbf{A}(\mathbf{r}, t) \) potential. For a single particle of mass \( m \) and charge \( q \) under a static potential \( V(\mathbf{r}) \), the Hamiltonian reads

\[
H = \frac{1}{2m}(\mathbf{p} - q \mathbf{A}(\mathbf{r}, t))^2 + V(\mathbf{r}) + qU(\mathbf{r}, t).
\]

The relationship between potentials and the electric \( \mathbf{E}(\mathbf{r}, t) \) and magnetic \( \mathbf{B}(\mathbf{r}, t) \) fields are

\[
\mathbf{E}(\mathbf{r}, t) = -\partial_t \mathbf{A}(\mathbf{r}, t) - \nabla U(\mathbf{r}, t) \tag{2}
\]

\[
\mathbf{B}(\mathbf{r}, t) = \nabla \times \mathbf{A}(\mathbf{r}, t). \tag{3}
\]

Gauge transformations are defined such that they preserve the electric and magnetic fields

\[
\mathbf{A}'(\mathbf{r}, t) = \mathbf{A}(\mathbf{r}, t) + \nabla \chi(\mathbf{r}, t) \tag{4}
\]

\[
U'(\mathbf{r}, t) = U(\mathbf{r}, t) - \frac{\partial}{\partial t} \chi(\mathbf{r}, t),
\]

where \( \chi(\mathbf{r}, t) \) is the scalar gauge transformation function.

A. Dipole-moment approximation (DMA)

In cases where the EM field varies little on the scale of the system taken to be centered around \( \mathbf{r} = 0 \) a gauge transformation is sought that would render \( \mathbf{A}'(\mathbf{r}, t) = 0 \) in the region around \( \mathbf{r} = 0 \). Assuming that for external radiation \( U(\mathbf{r}, t) = 0 \), this is achieved by the Göppert-Mayer gauge transformation \( \chi = -\mathbf{r} \cdot \mathbf{A}(0, t) \) \cite{28}

\[
A'_i(\mathbf{r}, t) = A_i(\mathbf{r}, t) - A_i(0, t) = \mathbf{r} \cdot \nabla A_i(\mathbf{r}, t)|_{\mathbf{r}=0} + \ldots \tag{5}
\]

\[
U(\mathbf{r}, t) = -\mathbf{r} \cdot \mathbf{E}(0, t). \tag{6}
\]

Thus, we can obtain \( \mathbf{A}'(\mathbf{r}, t) = 0 \) by neglecting the derivatives of the old vector potential. This leads to the well-known DMA Hamiltonian

\[
H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) - \mathbf{d} \cdot \mathbf{E}(0, t). \tag{7}
\]

Written in terms of an EM field, the DMA Hamiltonian is evidently gauge-invariant.

A striking feature of the DMA is that operators retain their physical meaning. As an important example, we look at the momentum. The canonical momentum is derived from the Lagrangian

\[
L = \frac{1}{2}m\dot{\mathbf{r}}^2 - V(\mathbf{r}) + q \mathbf{\dot{r}} \cdot \mathbf{A}(\mathbf{r}, t) - qU(\mathbf{r}, t) \tag{8}
\]

via \( p = \partial L/\partial \dot{r} \). Due to the fact that \( \mathbf{A}'(\mathbf{r}, t) = 0 \), the canonical momentum in the new gauge is equal to the mechanical momentum \( m\mathbf{\dot{r}} \).
B. Electric field coupling (EFC) Hamiltonian

In analogy with the DMA, a transformation function \( \chi = -r \cdot A(r, t) \) can be used\([42]\), yielding new potentials
\[
A'(r, t) = -(r \cdot \nabla)A(r, t) - r \times B(r, t) \tag{9}
\]
\[
U'(r, t) = -d \cdot E(r, t). \tag{10}
\]
As expected, the new scalar potential has the dipole-like form as that resulting from the Göppert-Mayer transformation, but now with a position-dependent electric field. However, the vector potential does not vanish and, thus, canonical and mechanical momenta now differ by
\[
p - m\dot{r} = q \{- (r \cdot \nabla)A(r, t) - r \times B(r, t)\}. \tag{11}
\]
However, for sufficiently localized charges and a sufficiently smooth vector potential it may be permissible to disregard the right hand side of Eq. (11), resulting in new potentials \( A'(r, t) = 0 \) and \( U'(r, t) = -d \cdot E(r, t) \), with the concomitant benefits of equality of momenta. We call this the Electric Field Coupling (EFC) approximation, which in contrast to DMA retains the spatial dependence of the electric field.

The mechanical momentum is indeed important, since it is a form-invariant operator\([27,43]\). As such, its eigenvalues are independent of the gauge, and thus represent physical quantities. On the other hand, the canonical momentum is not form-invariant. This is unfortunate, since the canonical momentum is typically used to perform calculations –in perturbation theory, mean values of operators, etc. However, we have seen that, in the case of the DMA, the canonical and mechanical momenta coincide, bestowing full physical meaning to the former, and to the calculations done with it. It should be understood that the requirement \( A'(r, t) = 0 \) in an extended region of space is a very stringent one, for it demands the magnetic field be zero, in violation to Maxwell’s equations for a propagating field.

III. THE VECTOR POTENTIAL OF TWISTED LIGHT

Let us now discuss gauge transformations for TL. In mathematical terms, the vector potential of a monochromatic TL beam in cylindrical coordinates \( \{r, \varphi, z\} \), can be described by \( A = A_r \hat{r} + A_\varphi \hat{\varphi} + A_z \hat{z} \) with components \([7,44]\)
\[
A_r(r, t) = F_{q_r,\ell}(r) \cos[(\omega t - q_z z) - (\ell + \sigma)\varphi] \\
A_\varphi(r, t) = \sigma F_{q_r,\ell}(r) \sin[(\omega t - q_z z) - (\ell + \sigma)\varphi] \\
A_z(r, t) = -\frac{q_r}{q_z} F_{q_r,\ell}(r) \sin[(\omega t - q_z z) - (\ell + \sigma)\varphi], \tag{12}
\]
with frequency \( \omega \), and wave vectors \( q_z \) and \( q_r \), related by \( q_z^2 + q_r^2 = (n\omega/c)^2 \), \( n \) being the index of refraction of the medium. This vector potential satisfies the Coulomb gauge condition \( \nabla \cdot A(r, t) = 0 \) and the vectorial Helmholtz equation.\([45] \)

The circular polarization of the field, given by vectors \( \epsilon_\sigma = e^{i\sigma\varphi} (\hat{x} + i\sigma \hat{y}) = \hat{x} + \sigma i \hat{y} \), is singled out with the variable \( \sigma \), which yields left(right-)handed circular polarization for the values \( \sigma = 1(-1) \). The OAM of the TL beam per photon is \( h\ell \), where the integer \( \ell \) is the so-called topological charge. The radial profile of the beam \( F_{q_r,\ell}(r) \) is a Bessel function: \( F_{q_r,\ell}(r) = A_0 J_\ell(q_r r) \), with \( A_0 \) being the amplitude of the potential. Note that \( 1/q_r \) is a measure of the beam waist.

Figure 1 shows the beam profile \( F_{q_r,\ell}(r) \) for non-vortex fields \((\ell = 0)\) and TL \((\ell = 1, 2)\).

In the paraxial approximation when \( q_r q_z \ll 1 \) the \( z \)-component of the vector potential is disregarded. This case has been extensively used in the literature\([1,3,6,12,38,40,46,48]\). The vector potential in the paraxial approximation \( A^{pa}(r, t) \) reads
\[
A^{pa}(r, t) = A_r(r, t) \hat{r} + A_\varphi(r, t) \hat{\varphi}. \tag{13}
\]
Here, the profile function \( F_{q_r,\ell}(r) \) can also be of the Laguerre-Gaussian type\([8]\), satisfying the paraxial Helmholtz equation.

IV. A HEURISTIC DERIVATION OF THE TWISTED LIGHT - MATTER INTERACTION

In this section, following the spirit of the DMA, we derive a gauge transformation that captures the essential features of TL, and at the same time retains the advantages of the DMA, e. g. the equality of mechanical and canonical momenta. The derivation is intended to be intuitive and self-evident, and is only done for a paraxial vector potential \([Eq. (13)]\). A formal analysis leading to the same results is given in Sec.\([\hat{\n}] \) where the more general form of the vector potential \([Eq. (12)] \) is used.
A. Interaction off the phase singularity

It is instructive to first note what happens when the interaction takes place far from the phase singularity, i.e., in a region where the TL radial profile function does not vanish. An example is the interaction of TL with a small quantum dot displaced from the beam axis and centered at \( r_0 = (r_{max}, \phi_0, z_0) \), where \( r_{max} \) is the position of maximum intensity of the field. In this region, the beam intensity varies little and, most importantly, the radial profile can be approximated by a constant. Then, a gauge transformation of the type \( \chi = -r \cdot A(r_0, t) \) can be used such that \( \nabla \chi = -A(r_0, t) \). The vector potential in the new gauge is \( A'(r_0, t) = 0 \). This leads to a DMA-like Hamiltonian, where the TL-matter interaction is described by \(-d \cdot E(r_0, t)\).

B. Interaction close to the phase singularity

Let us next consider a planar structure of size smaller than the beam waist \((q,r \ll 1)\), such as a quantum disk or a quantum dot centered at \( r = 0 \). The vector potential interacting with the structure is that of Eq. (13), with the radial profile approximated by \( F_{q,\ell}(r) = \alpha_{\ell}(q,r)^{\ell} \), with \( \alpha_{\ell} \) a constant. To simplify the expressions, we will use in this section the case \( \ell > 0 \).

Note that the vector potential [Eq. (13)] at \( r = 0 \) is zero, and thus, within the DMA there would be no interaction whatsoever. Motivated by the EFC Hamiltonian, we try a gauge transformation function of the form

\[
\chi(r, t) = -\frac{1}{\beta} r_{\perp} \cdot A^{pa}(r, t),
\]

where we have defined a two-dimensional in-plane position vector \( r_{\perp} = r \hat{x} + y \hat{y} \) out of the 3D vector \( r \), and added a constant prefactor \( 1/\beta \) to be determined later. The EFC gauge is recovered for \( \beta = 1 \). The vector potential in the new gauge, from Eq. (1), is calculated to

\[
A^{pa}(r, t) = \left( 1 - \frac{\ell + 1}{\beta} \right) A^{pa}_{\perp}(r, t) \hat{r} \\
+ \left( 1 - \frac{\sigma \ell + 1}{\beta} \right) A^{pa}_{\parallel}(r, t) \hat{\phi} \\
- \frac{q_{z} F_{q,\ell}(r)}{\beta} \frac{\sigma \ell + 1}{\beta} \sin(\Omega) \hat{z},
\]

where \( \Omega = (\omega t - q_{z} z - (\ell + \sigma) \phi) \).

When \( \sigma = 1 \) the in-plane components \( A^{pa}_{\perp} \) and \( A^{pa}_{\parallel} \) of the new vector potential vanish for \( \beta = \ell + 1 \). In this case, the remaining component \( A^{pa}_{\parallel} \) should be disregarded because it is proportional to \((q,r)^{\ell + 1}\). This is consistent with keeping terms up to order \((q,r)^{\ell}\), and therefore on the same footing as doing the paraxial approximation for \( \sigma = 1 \). As a result \( A^{pa}(r, t) = 0 \). We will refer to the case \( \beta = \ell + 1 \) as the TL gauge. The Hamiltonian then reads

\[
H = \frac{p^{2}}{2m} + V(r) - \frac{1}{\ell + 1} d_{\perp} \cdot E^{pa}(r, t).
\]
parameter $q_\ell / q_z$. The electric field acquires a small $z$-component which is of first order in $q_\ell / q_z$ and additionally it is proportional to $(q_\ell r)^{[\ell]+1}$ and thus decreases faster for $r \to 0$ than the in-plane components. Thus, these corrections are negligible in the framework of the paraxial approximation and the fields agree.

In the anti-parallel class $[\text{Sign}(\ell) \neq \text{Sign}(\sigma)]$, on the other hand, the vector potential in paraxial approximation leads to a pure in-plane electric field while the magnetic field has a non-vanishing $z$-component. This $z$-component contains the small parameter $q_\ell / q_z$, however the radial dependence is proportional to $(q_\ell r)^{[\ell]-1}$, thus at small $r$ it dominates over the in-plane components. Moreover, when looking at the fields obtained from the full vector potential we note that here also the electric field has a $z$-component with the same radial dependence. Therefore, for $|\ell| = 1$ there are non-vanishing electric and magnetic fields at $r = 0$ pointing in the $z$-direction.

In the paraxial approximation a longitudinal component for the magnetic field is obtained while the analogous component for the electric field does not exist. This is a clear indication that this approximation is not applicable in the anti-parallel class when one is interested in beam properties close to the center of the beam. Indeed, a careful look at the $z$-component of the potential in Eq. (12) reveals that already there the small factor $q_\ell / q_z$ is counterbalanced by a $r$-dependence which is one order lower than for the in-plane components and therefore dominates close to $r = 0$.

For angular momenta $|\ell| \geq 2$ the magnetic field in the anti-parallel class has an additional correction which is of second order in $q_\ell / q_z$ but which has a $r$-dependence proportional to $(q_\ell r)^{|\ell|-2}$. For sufficiently small radii this is the dominant contribution to the fields. Thus, in this case close to the center the beam is dominated by the magnetic field. This holds in particular for the case $|\ell| = 2$, in which there is a non-vanishing in-plane magnetic field at the beam center while the electric field vanishes. This is again an indication that the EFC Hamiltonian is not applicable since with such a Hamiltonian the interaction with matter is described only in terms of the electric field.

| $\ell > 0$, $\sigma = 1$ | $\ell > 0$, $\sigma = -1$ |
|-------------------------|-------------------------|
| $E(r,t)$ $\omega F_{q_\ell}(r)$ | $\hat{r} - \hat{\phi}$ + $\frac{q_\ell}{q_z} q_\ell r \hat{z}$ | $\hat{r} + \hat{\phi}$ - $\frac{q_\ell}{q_z} q_\ell r^{-1} \hat{z}$ |
| $\tilde{B}(r,t)$ $q_\ell F_{q_\ell}(r)$ | $1 + (\frac{q_\ell}{q_z})^2 (1 + \ell)$ | $-1 - (\frac{q_\ell}{q_z})^2 (1 - \ell)$ |
| $\hat{B}_x(r,t)$ | $\hat{B}_y + \hat{\phi}$ | $-\hat{B}_y + \hat{\phi}$ |
| $\hat{B}_z(r,t)$ | $-2\ell \frac{q_\ell}{q_z} (q_\ell r)^{-1} \hat{z}$ |

TABLE I. Electric and magnetic field amplitudes near $r = 0$ calculated from the full vector potential in Eq. (12). The factors $q_\ell$, $\omega$, and $F_{q_\ell}(r)$ are included in the denominator in the first column.

| Paraxial approximation |
|-------------------------|
| $\ell > 0$, $\sigma = 1$ | $\ell > 0$, $\sigma = -1$ |
| $E^{\text{par}}(r,t)$ $\omega F_{q_\ell}(r)$ | $\hat{r} - \hat{\phi}$ | $\hat{r} + \hat{\phi}$ |
| $\tilde{B}^{\text{par}}(r,t)$ $q_\ell F_{q_\ell}(r)$ | $\hat{B}_x(r,t)$ | $-\hat{B}_y + \hat{\phi}$ |
| $\hat{B}_z(r,t)$ | $-2\ell \frac{q_\ell}{q_z} (q_\ell r)^{-1} \hat{z}$ |

TABLE II. Same as in Table I but in the paraxial approximation Eq. (13).

Some research articles in the topics of highly focused TL and azimuthally/radially-polarized fields report similar findings to ours. Paraxial beams of TL can be focused using high-NA lenses, as experimentally demonstrated in Refs. [49] and [50]. The theoretical analysis of focusing, based entirely on electric and magnetic fields, can be done using the formalism by Wolf [51], and the results [49] [50] show important similarities with the field patterns presented in Fig. 2. Azimuthally- and radially-polarized fields are a special class of TL fields. The field patterns of azimuthally/radially-polarized non-paraxial Bessel beams presented by Ornigotti et al. [24] are also in agreement with our findings. Regarding the magnitude of the fields near $r = 0$ Zurita-Sánchez et al. [26] have shown that, for the strongly focused azimuthally-polarized beam they studied, the magnetic interaction overcomes the electric interaction near the phase singularity; recently, their findings have been corroborated by the theoretical study of Klimov et al. [41] in the case of...
focused Laguerre-Gaussian beams. Finally, in their research on highly-focused TL beams, Monteiro et al. [52], Iketa et al. [49] and Klimov et al. [41] report that interesting effects only occur when \( \ell = 1, 2 \) and \( \sigma = -1 \). The overall similarities are no coincidence, for the vector potential Eq. (12) —in contrast to Eq. (13)— shares with the aforementioned non-paraxial beams the important feature of having a non-negligible \( z \)-component, which we have shown to give rise to the described features.

We are now in a position to clarify the findings in the heuristic derivation of the TL-matter coupling shown in Sec. IV. There it was assumed that there is no \( z \)-component in the vector potential. From Table 1 we see that the \( z \)-component of the fields are negligible only in the parallel class. In the anti-parallel class they are proportional to \( (q, r)^{-1} F_{q, \ell}(r) \). Because for \( r \to 0 \) the magnetic field cannot be neglected compared to the electric field, we were not able to derive a dipole moment like Hamiltonian. In other words a Hamiltonian representation given solely in terms of the electric multipoles, such as \( -(1/\beta) \mathbf{d} \cdot \mathbf{E}(r, t) \), is insufficient to describe the TL-matter interaction with very small systems at the phase singularity.

VI. FORMAL DERIVATION OF THE TL-MATTER INTERACTION: THE POINCARÉ GAUGE

The use of the gauge transformation function \( \chi(r, t) \) found in Sec. IV can be motivated using formal arguments. In the following we use the more general form Eq. (12) for the vector potential in the Coulomb gauge.

For charged particles localized around the same center, a Power-Zienau-Woolley (PZW) transformation can be done using the function

\[
\chi(r, t) = - \int_0^1 r \cdot A(\mathbf{ur}, t) du ,
\]

where \( A(\mathbf{ur}, t) \) is given in the Coulomb gauge. This is the generalization to inhomogeneous fields of the Göppert-Mayer transformation (DMA), and leads to the so-called Poincaré gauge [28, 29]. The focus of our work has been the study of planar systems. Therefore, if we consider a charge distribution mainly extended in the \( x-y \) plane for a fixed \( z \), the quantity \( \mathbf{ur} \) scales only in the \( \perp \) component with \( \mathbf{ur} \cong (ur, \varphi, z) \) (see e.g. Ref. [28]). Defining \( \mathbf{r} = \mathbf{r}_\perp + z \mathbf{z} = \mathbf{r}_\perp + z \mathbf{z} \), the gauge function reads

\[
\chi(r, t) = - \int_0^1 \mathbf{r}_\perp \cdot A(\mathbf{ur}, \varphi, z; t) du
- \int_0^1 z A_z(\mathbf{ur}, \varphi, z; t) du .
\]

For small systems \( (q, r \ll 1) \) the spatial dependence can be approximated with \( F_{q, \ell}(r) \approx \alpha_v(q, r)^{\ell} \), which leads to \( F_{q, \ell}(ur) \approx u^\ell F_{q, \ell}(r) \). With these simplifications, we evaluate the integrals Eq. (18), and obtain

\[
\chi(r, t) = - \frac{1}{|\ell| + 1} r_\perp \cdot A(r, t) - \frac{1}{|\ell + \sigma| + 1} z A_z(r, t) .
\]

The in-plane part of the transformation function \( \chi(r, t) \) is exactly the same as we got in Sec. IV. In addition, there is a new term arising from the non-vanishing \( z \)-component of the vector potential. Note that we have neither required \( A\'(r, t) = 0 \) in the new gauge, nor have we neglected \( A_z(r, t) \). Additionally, for non-vortex fields \( (\ell = 0) \) having no \( z \)-component our result coincides with that of the EFC Hamiltonian. It is worth mentioning that any gauge transformation function can be postulated and used to cast the potential in suitable forms. Here we have shown that the TL gauge function stems from a Poincaré transformation for planar structures similar to the PZW transformation, which is intended as a motivation for the use of the new \( \chi(r, t) \) Eq. (19). Thus, the TL gauge can also be applied to other more general structures (with varying degrees of accuracy or usefulness).

The Poincaré gauge shows that the natural extension of the DMA to the case of TL beams is slightly different from the plain EFC Hamiltonian. Because of the generalized use of EFC Hamiltonian, it is worth exploring further its connection to our result. To this end, let us simple postulate a general gauge transformation of the form

\[
\chi_\beta(r, t) = - \frac{1}{\beta_r} r_\perp \cdot A(r, t) - \frac{1}{\beta_z} z A_z(r, t) ,
\]

where \( \beta_\ell \) is any number. Clearly, we can recover the EFC Hamiltonian setting \( \beta_\ell = 1 \), and the TL gauge by \( \beta_r = |\ell| + 1 \) and \( \beta_z = |\ell + \sigma| + 1 \). In the following, to simplify the discussion, we will only consider the case of \( \ell > 0 \) and polarization \( \sigma = \pm 1 \), for it has already been shown that there are no essential differences for the case with negative \( \ell \).

From Eqs. 11, explicit expressions can be given for the new scalar potential in the new gauge

\[
U'(r, t) = - \frac{1}{\beta_r} r_\perp \cdot \mathbf{E}(r, t) - \frac{1}{\beta_z} z E_z(r, t) ,
\]

Obviously in the scalar potential we regain a dipole moment type structure of the Hamiltonian. The new vector potential is
\[
A'_r(r, t) = \beta_r - (1 + \ell) \beta_r A_r(r, t) + \frac{2 - \sigma (\ell + \sigma) \ell!}{\beta_r (\ell + \sigma)!} \left( \frac{q_z}{q_r} \right)^2 (q_z)(q_r)^{\sigma-1} A_r(r, t) \\
A'_\varphi(r, t) = \beta_r - (1 + \ell \beta_r) A_\varphi(r, t) - \sigma \frac{2 - \sigma (\ell + \sigma) \ell!}{\beta_r (\ell + \sigma)!} \left( \frac{q_z}{q_r} \right)^2 (q_z)(q_r)^{\sigma-1} A_r(r, t) \\
A'_z(r, t) = \left[ 1 - \frac{1}{\beta_z} + \sigma \frac{2\ell (\ell + \sigma) \ell!}{\beta_r \ell!} \left( \frac{q_z}{q_r} \right)^2 (q_r)^{-\sigma} \right] A_z(r, t) - \sigma \frac{2 - \sigma \ell!}{\beta_z (\ell + \sigma)!} q_z (q_z)(q_r)^{\sigma} A_r(r, t),
\]

(22) (23) (24)

We will discuss the vector potential for the different cases in the following. We remind that \( A_r(r, t) \) and \( A_\varphi(r, t) \) are proportional to \((q_r)^{\ell}\) while \( A_z \propto (q_r)^{\ell+\sigma} \).

### A. Vector potential in the parallel class

We first examine the new vector potential in the parallel class, i.e. \( \text{Sign}(\ell) = \text{Sign}(\sigma) \) or more explicitly \( \sigma = 1 \). The results are a direct extension to those found by the heuristic derivation in Sec. IV.

#### 1. The EFC gauge

In the EFC gauge we set \( \beta_i = 1 \) for all \( i \). A quick inspection of Eqs. (22)-(24) reveals no divergent behavior close to the phase singularity, such as a term like \((q_r)^{-1}\) would be. Moreover, each component of the vector potential contains a term proportional to the small quantities \((q_z, z)\). For this reason, it is admissible to simplify the expressions to

\[
A'_r(r, t) = -\ell A_r(r, t) \\
A'_\varphi(r, t) = -\ell A_\varphi(r, t) \\
A'_z(r, t) = 2(1 + \ell) \left( \frac{q_z}{q_r} \right)^2 A_z(r, t).
\]

(25) (26) (27)

We see that the vector potential in the EFC gauge grows with \( \ell \), as was already noticed in Sec. IV. This impacts directly on the difference between canonical and mechanical momentum \( p - m \dot{r} = q A(r, t) \), which also grows with \( \ell \). Therefore, when the EFC gauge is applied to high-\( \ell \) TL beams at the phase singularity and the canonical momentum instead of the mechanical momentum is used in calculations, a significant error may be introduced.

#### 2. The TL gauge

In the TL gauge we set \( \beta_r = \ell + 1 \) and \( \beta_z = \ell + \sigma + 1 = \ell + 2 \). Using the same approximation as before, namely neglecting terms including \((q_z, z)\), the expressions simplify to

\[
A'_r(r, t) = 0 \\
A'_\varphi(r, t) = 0 \\
A'_z(r, t) = \left[ \frac{1 + \ell}{2 + \ell} + 2 \left( \frac{q_z}{q_r} \right)^2 \right] A_z(r, t).
\]

(28) (29) (30)

The first thing to notice is that the components \( A'_r \) and \( A'_\varphi \) of the new vector potential are zero as we have already found in Sec. IV. Therefore, in the Hamiltonian

\[
H = \frac{p^2}{2m} + V(r) - \frac{1}{\ell + 1} d_1 \cdot E(r, t) - \frac{1}{\ell + 2} d_z E_z(r, t) - \frac{q}{m} p_z A'_z(r, t) + \frac{q^2}{2m} A'_z^2(r, t),
\]

(31)

the in-plane TL-matter interaction can be expressed solely by a dipole like term \(-\frac{q}{m} p_z A'_z(r, t)\) with a prefactor different to the EFC Hamiltonian. For the \( z \)-component we have both a dipole like term, but also a term \(-\frac{q^2}{2m} A'_z^2(r, t)\) which still contains the vector potential. We point out that \( q^2/(2m) A'_z^2(r, t) \) and may be safely disregarded.

It is interesting to also compare again the canonical and mechanical momenta, which are derived from the Lagrangian

\[
L = \frac{1}{2} m \dot{r}^2 - V(r) + \frac{1}{\ell + 1} d_1 \cdot E(r, t) + \frac{1}{\ell + 2} d_z E_z(r, t) + q \dot{z} A'_z(r, t),
\]

(32)

leading to the following difference between momenta:

\[
p - m \dot{r} = q A'_z(r, t) \dot{z}.
\]

(33)

Also here the canonical and mechanical momenta are the same for the in-plane components and only in the \( z \)-component a difference in the momenta arise.

Let us now consider what happens in situations of experimental and application interest. We first address the situation when the interaction with the system only occurs through the in-plane components of the field, for example in the selective excitation of heavy holes in a quantum dot. Then, the TL-matter interaction reads

\[
H_{T L-matter} = -\frac{q}{\ell + 1} d_1 \cdot E(r, t)
\]

and is modeled by electric multipoles only with all the benefits of a DMA. Effectively we end up in the desirable situation where the vector potential is eliminated, as also shown in Sec. IV.
Next, consider the case where the system interacts with the \( z \)-component of the field, for example in intersubband transitions\cite{19} or the excitation of light holes. Here, the electric multipoles are accompanied by a magnetic term arising from the non-vanishing \( z \)-component vector potential. However, since no atypical behavior near the phase singularity occurs, it is expected that the electric interaction is larger than the magnetic one as usually happens. One could then safely only retain the electric multipolar term, and possibly neglect the difference between momenta. Therefore for the parallel class a Hamiltonian with only electric dipole moment terms having the correct prefactors can describe the TL-matter interaction at the phase singularity.

2. The TL gauge

In the TL gauge, we again put \( \beta_r = \ell + 1 \) and \( \beta_z = \ell + \sigma + 1 = \ell \). With this, the vector potential reads:

\[
A'_r(r, t) = 2(\ell - 1) \left( \frac{q_r}{q_z} \right)^2 \frac{q_z}{(q_r r)^2} A_r(r, t)
\]

\[
A'_\varphi(r, t) = 2 \frac{\ell}{\ell + 1} A_r(r, t) + 2(\ell - 1) \left( \frac{q_r}{q_z} \right)^2 \frac{q_z}{(q_r r)^2} A_r(r, t)
\]

\[
A'_z(r, t) = \left[ \frac{1}{2\ell} \left( \frac{q_z}{q_r} \right)^2 (q_r r)^2 \right] A_z(r, t) + 2 \frac{q_r}{q_z} \frac{q_z}{q_r r} A_r(r, t).
\]

Like above in the EFC gauge for the anti-parallel class, the in-plane components the vector potential exhibits new terms containing \((q_r r)^{-2}\), always accompanied by \((q_z z)^{-1}\), indicating that the magnetic field contribution can overcome the electric one. It is also interesting, that even far from the phase singularity, the in-plane term \( A'_\varphi \) does not vanish.

Let us study this in more detail using as an example the excitation of a quantum dot placed at the beam axis by a TL beam and energy close to the QD band-gap. Based on energy considerations, we neglect the \( z \)-component of the interaction, and also the terms proportional to \( A(r, t)^2 \). Then, the Hamiltonian reduces to

\[
H \simeq \frac{p^2}{2m} + V(r) - \frac{1}{\ell + 1} \mathbf{d}_\perp \cdot \mathbf{E}(r, t) - \frac{q}{2m} [\mathbf{p}_\perp \cdot \mathbf{A}'_\perp(r, t) + A'_\perp(r, t) \cdot \mathbf{p}_\perp].
\]

We note that the angular component of the momentum vector reads \((p)_\varphi = (1/\ell) p_\varphi\), where \( p_\varphi = \partial L/\partial \varphi \).\cite{53} Though there is a dipole-type Hamiltonian, clearly the in-plane vector potential remains in the Hamiltonian. We wonder how electric and magnetic contributions compare to each other. Let us specifically consider the case \( \ell = 2 \). Then, the electric multipolar term is proportional to \( r(q_r r)^2 \). On the other hand, the magnetic term in Eq.\cite{40} is proportional to \( p(q_r r)^3 \). If we assume that momentum and position vector are proportional to each other, as it is so in the DMA \((p = -i(m/\hbar)[r, H_0])\), it becomes clear that one should not a priori neglect the magnetic interaction, for it may be comparable or even larger the electric interaction, in particular at the phase singularity.

When the \( z \)-component of the fields become also important, it is clear that also here the vector potential remains in the Hamiltonian. In summary, in the anti-parallel class the TL-gauge transformation is not advantageous.

B. Vector potential in the anti-parallel class

For the anti-parallel class, we already found that a description with electric field only is not sufficient. Still, we can gain valuable insights from studying the anti-parallel case with \( \text{Sign}(\ell) \neq \text{Sign}(\sigma) \), namely we set \( \sigma = -1 \).

1. The EFC gauge

If we put \( \beta_i = 1 \) for the EFC gauge, the vector potential in the new gauge reads

\[
A'_r(r, t) = -\ell A_r(r, t)
\]

\[
+ 2(\ell - 1) \ell \left( \frac{q_r}{q_z} \right)^2 \frac{q_z}{(q_r r)^2} A_r(r, t)
\]

\[
A'_\varphi(r, t) = \left[ \ell + 2 \frac{\ell}{\ell + 1} \right] A_r(r, t)
\]

\[
+ 2(\ell - 1) \ell \left( \frac{q_r}{q_z} \right)^2 \frac{q_z}{(q_r r)^2} A_r(r, t)
\]

\[
A'_z(r, t) = \left[ -\frac{1}{2\ell} \left( \frac{q_z}{q_r} \right)^2 (q_r r)^2 \right] A_z(r, t)
\]

\[
+ 2 \frac{q_r}{q_z} \frac{q_z}{q_r r} A_r(r, t).
\]

In contrast to what happens in the parallel class, the vector potential exhibits new terms containing \((q_r r)^{-n}\). Close to the phase singularity, the magnetic interaction resulting from these terms may be comparable or even surpass the electric interaction. This is in agreement with previous results for highly focused beams, where a magnetic field contribution stronger than the electric field contribution at the phase singularity was found.\cite{26,41}
VII. CONCLUSIONS

We have studied the TL-matter interaction close to the beam axis. In contrast to conventional light beams, twisted light has a phase singular at the point $r = 0$, and a strong intermixing between polarization and OAM. We distinguished the TL beams into two topologically different classes, namely the parallel class where circular polarization and OAM momentum have the same sign and the anti-parallel class where the signs of polarization and OAM momentum differ.

To obtain a Hamiltonian which includes the EM fields instead of the potentials, we suggested to use a new gauge, the TL gauge. For the parallel class, the TL gauge leads to a Hamiltonian which has a dipole-type structure, but a different prefactor. For in-plane problems it takes the simple form $H_{TL-matter} = -\frac{1}{|r|+1} \mathbf{d}_\perp \cdot \mathbf{E}(r, t)$. The prefactor is mandatory to describe the correct interaction and to achieve the identity of canonical and mechanical momentum. The origin of the prefactor in the TL gauge is the vortex, which exists at the phase singularity. For the anti-parallel class we showed that the TL gauge, which casts the Hamiltonian at least partly into electric fields, is not advantegous as the vector potential cannot be eliminated nor neglected. Because in the anti-parallel class magnetic effects cannot be neglected compared to the electric ones, the Hamiltonian should include magnetic as well as electric terms, and their relative strength must be analyzed in the particular problem at hand.

We compared the TL gauge to the more common EFC Hamiltonian and found that the EFC gauge is not useful at all to describe the TL-matter interaction at the beam axis. We have also pointed out that the use of the paraxial approximation close to the phase singularity is misleading and should be avoided at least in the anti-parallel beam class. We shortly discussed the TL-matter interaction at the beam maximum, where it should be safe to use a DMA-like Hamiltonian.

In comparison to other known gauges, like the Poincaré-gauge or the multipolar gauge, the TL gauge offers the same advantages as the DMA for TL in the parallel class: In contrast to the Pioncaré-gauge, the TL gauge can be simply evaluated and leads to explicit formulas. For in-plane problems $H_{TL-matter}$ contains only the electric field, which makes it manifestly gauge invariant and secures the physical meaning of the momentum operator. Furthermore, it contains all the higher order electric field couplings like coupling to quadrupole terms in a compact, appealing form.

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