Quantized toroidal dipole eigenvalues in nano-systems

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Abstract. The parity violation in nuclear reactions led to the discovery of the new class of toroidal multipoles. Since then, it was observed that toroidal multipoles are present in the electromagnetic structure of systems at all scales, from elementary particles, to solid state systems and metamaterials. The toroidal dipole $T$ (the lowest order multipole) is the most common. This corresponds to the toroidal dipole operator $\hat{T}$ in quantum systems, with the projections $\hat{T}_i$ ($i = 1, 2, 3$) on the coordinate axes. These operators are observables if they are self-adjoint, but, although it is commonly discussed of toroidal dipoles of both, classical and quantum systems, up to now no system has been identified in which the operators are self-adjoint. Therefore, in this paper we use what are called the “natural coordinates” of the $\hat{T}_3$ operator to give a general procedure to construct operators that commute with $\hat{T}_3$. Using this method, we introduce the operators $\hat{p}^{(k)}$, $\hat{p}^{(k_1)}$, and $\hat{p}^{(k_2)}$, which, together with $\hat{T}_3$ and $\hat{L}_3$, form sets of commuting operators: $(\hat{p}^{(k)}, \hat{T}_3, \hat{L}_3)$ and $(\hat{p}^{(k_1)}, \hat{p}^{(k_2)}, \hat{T}_3)$. All these theoretical considerations open up the possibility to design metamaterials that could exploit the quantization and the general quantum properties of the toroidal dipoles.

1. Introduction

Toroidal moments first emerged as a new field of research in the context of nuclear physics, when Zeldovich introduced in 1957 a new type of electromagnetic interaction to explain parity nonconservation in $\beta$-decays \cite{1}:

$$\hat{H}_\beta \sim \mathbf{S} \cdot \mathbf{J}^{ext} = \mathbf{S} \cdot (\nabla \times \mathbf{H}^{ext})$$ (1)

($\mathbf{S}$ is the spin of the particle, $\mathbf{J}^{ext}$ is the external current, and $\mathbf{H}^{ext}$ is the external magnetic field). Since neither electric nor magnetic multipoles lead to an interaction of the type (1), this novel charge configuration came to be known as "anapole" and it was visualized as a toroidal solenoid with a current flowing along the poloidal lines (as in Fig. 1), which produces a magnetic field localized inside the torus, while the external electromagnetic field of the configuration is zero.

In 1997, decades after Zeldovich published his pioneering article \cite{1}, the anapole moment was measured by Wood \textit{et al.} by determining the amplitude of the transition between $6S$ and $7S$ states in $^{133}\text{Cs}$ \cite{35}.

In the late 1970s, Dubovik \textit{et al.} expanded the concept of the anapole to classical electrodynamics and introduced a new family of multipoles, that he called "polar toroidal multipole moments" \cite{2,3}. Like the electric and magnetic moments, toroidal moments form an
Fundamental symmetry considerations explain the need for this new family of multipoles. For example, the electric dipole is odd under spatial inversion and even under time reversal, while the magnetic dipole is odd under time reversal and even under spatial inversion. For a complete picture, one needs to include dipole moments which are even or odd under both transformations and these are the axial and polar toroidal dipoles [4].

Although overlooked for a long time, it has been realized that the toroidal moments and anapole configurations represent an important tool to describe the properties of systems at all scales, from particle physics to the physics of macroscopic systems and this new field expanded rapidly [5, 6]. Nuclear anapole moments were explored thoroughly in a series of articles [9, 6, 7, 8, 12, 10], focusing on both the theoretical implications, as well as the experimental techniques. Probably one of the most remarkable discoveries in this field is that massive Majorana particles can possess only toroidal moments, which in turn lead to the idea that dark matter particles could be characterized by the anapole [9, 10, 11, 12].

In solid state physics, toroidal ordering was first studied theoretically by Charles Kittel [13] and it indicates the existence of a new type of magnetoelectric effect. In the framework of condensed matter, toroidal moments are linked to another kind of order parameter known as toroidization (toroidal polarization). Media that exhibit macroscopic toroidization are called ferrotoroids and since they are expected to have promising technological applications (for example in data storage), it is crucial to investigate whether ferrotoroidicity is on an equal footing with the other ferroic states (ferroelectric, ferromagnetic) [17, 18, 19, 20, 21, 22, 23, 24]. On top of this, the toroidal moments were studied in relation to the antisymmetric magnetoelectric effect and it was shown that any bulk toroidization results in the emergence of an antisymmetric magnetoelectric tensor [14, 15, 16]. Moreover, a magnetoelectric effect was predicted in skyrmion crystals and it was quantified with the aid of spin toroidization [15].

Recently, anapole states have generated tremendous interest in the field of nanophotonics, optics and metamaterials and have great potential for a wide range of applications like lasers, sensing and nonscattering objects that may be used for their cloaking behaviour [25, 26, 27, 28]. It has even been proposed that since anapole states interact weakly with electromagnetic fields, they could be used to protect qubits from environmental disturbance [29].

The lowest order toroidal moment corresponding to a current distribution \( \mathbf{j}(\mathbf{r}) \) is a polar vector of components

\[
T_i = \frac{1}{10 \epsilon} \int_V \left[ r_i (\mathbf{r} \mathbf{j}) - 2 r^2 j_i \right] d^3 \mathbf{r}
\]  

where \( r \equiv |\mathbf{r}|, \ j \equiv |\mathbf{j}|, \ T \equiv |\mathbf{T}|, \) and \( i = 1, 2, 3 \) number the components of a vector on the three axes \( x, y, \) and \( z: \ \mathbf{T} \equiv (T_1, T_2, T_3), \ \mathbf{j} \equiv (j_1, j_2, j_3), \ \mathbf{r} \equiv (r_1, r_2, r_3) \equiv (x, y, z) \) [34]. The
electromagnetic interaction Hamiltonian
\[ \mathcal{H} \equiv \int \left( \rho \dot{\phi} - \frac{1}{c} j \mathbf{A} \right) d^3 r \]  
may be decomposed into multipoles interactions, leading to the term characterizing the interaction of the toroidal moment with the external fields \[34\]
\[ \mathcal{H}_{\text{tor}}(t) = -T(t) \left[ \nabla \times \nabla \times A^{\text{ext}}(\mathbf{r}, t) \right]_{r=0} \equiv -T(t) \left[ \frac{4\pi}{c} J^{\text{ext}}(\mathbf{r}, t) + \frac{1}{c} \dot{D}^{\text{ext}}(\mathbf{r}, t) \right]_{r=0}. \]  

To correctly predict the toroidal moments of quantum systems (particles, nuclei, or macroscopic systems), one has first to study the quantum operators corresponding to them and their basic mathematical properties.

The quantum operators which correspond to the classical toroidal moments (2) are \[30, 33\]
\[ \hat{T}_i \equiv \frac{1}{10mc} \sum_{j=1}^{3} (x_ix_j - 2r^2 \delta_{ij}) \hat{p}_j, \]  
where \( \hat{p}_j \equiv -i\hbar \partial / \partial x_j \) is the momentum operator along the \( j \) axis and \( m \) is the mass of the particle. We observe that the commutation relations \[33\]
\[ [\hat{T}_i, \hat{L}_j] = i\hbar \epsilon_{ijk} \hat{T}_k, \]  
amre satisfied, where \( \hat{L}_j \) is the projection of the angular momentum operator on the \( j \) axis. In \[33\] it was shown that in \( \mathbb{R}^3 \) space, \( \hat{T}_3 \) (and, equivalently, \( \hat{T}_1 \) and \( \hat{T}_2 \)) is a hypermaximal operator (admits several self-adjoint extensions).

The operator \( \hat{T}_3 \) has a specific “natural coordinate”, denoted by \( u \), such that
\[ \hat{T}_3 = -i\hbar \frac{\partial}{\partial u}, \]  
(notice that in \[33\] \( u \) had a different scale, namely \( \hat{T}_3 = -[i\hbar/(10mc)]\partial / \partial u \)). Starting from \( u \), one can form the so called “natural systems of coordinates” for the operator \( \hat{T}_3 \), like \((k, u, \phi)\) and \((k_1, k_2, u)\), as it will be explained in Section 2. In the natural systems of coordinates it is easy to construct operators that commute with \( \hat{T}_3 \), so one can form sets of commuting operators and find their eigenvectors and eigenvalues. Furthermore, we can translate the operators defined in the natural system of coordinates into operators acting on the \((x, y, z)\) coordinates and vice-versa.

2. Method
The main tools used in this paper, as in Ref. \[33\], are two natural sets of coordinates of the toroidal moment operator, which we shall present in this section to introduce the notations and make the paper easier to read.

2.1. The natural coordinates for the toroidal moment operator
In the following we shall focus on the operator \( \hat{T}_3 \). The analysis of \( \hat{T}_1 \) and \( \hat{T}_2 \) may be done in a similar fashion. According to Eq. (6), \([\hat{T}_3, \hat{L}_3] = 0\), so it is more convenient to write in cylindrical coordinates \[33\]
\[ \hat{T}_3 = -i\hbar \frac{10mc}{10mc} \left[ z\rho \frac{\partial}{\partial \rho} - (2\rho^2 + z^2) \frac{\partial}{\partial z} \right], \]  
\[ (8) \]
Figure 2: (a) The directions of the vector field $T_3$ (i.e., $t_3 \equiv T_3/T_3$) in a plane that contains the $z$ axis (the units on the axes are arbitrary). The vector field is tangent in every point to the continuous lines that represent the lines along which the “natural variable” $u$ vary. In (b) we show the range of $u$, as a function of $k$ (in arbitrary units): $u \in (-a(k), a(k))$.

where $\rho \equiv \sqrt{x^2 + y^2}$, $r = \sqrt{\rho^2 + z^2}$. We define the vector field $T_3$ by the relation

$$\hat{T}_3 \equiv -i\hbar T_3 \cdot \nabla.$$ (9)

We plot the directions of $T_3$ (i.e., $t_3 \equiv T_3/T_3$, where $T_3 \equiv |T_3|$) in Fig. 2, in a plane which contains the $z$ axis. We observe that $\hat{T}_3$ may be written as a derivative along the lines of this vector field, that is, along the continuous curves shown in the figure. This observation led to the introduction of the “natural” set of coordinates $(k, u, \phi)$ [33], in which $\hat{T}_3$ takes the form (7), whereas

$$k \equiv [\rho^2(z^2 + \rho^2)]^{1/4} \equiv \sqrt{\rho^2} \quad \text{and} \quad u \equiv -10mc \int_0^z \frac{dt}{\sqrt{t^4 + 4k^4}} = \pm 10mc \int_0^k \frac{dt}{\sqrt{-t^4 + k^4}}; \quad (10)$$

the curves in Fig. 2 correspond to $k(\rho, z) = \text{const}$.

The variable $u$ takes values in a finite interval $(-a(k), a(k))$, with [33]

$$a(k) = \frac{10mc}{4k} \frac{\Gamma \left(\frac{1}{4}\right) \Gamma \left(\frac{3}{4}\right)}{\Gamma \left(\frac{1}{2}\right)} = \frac{10mc}{k} C_a$$ (11)

and $C_a \approx 1.31103$. Notice that all the end points $-a(k)$ and $a(k)$ (for all $k$) correspond to the points ($z \to \infty, \rho = 0$) and ($z \to -\infty, \rho = 0$), respectively.

Beside $(k, u, \phi)$, we may define the set of coordinates $(k_1, k_2, u)$ by

$$k_1 = k \cos \phi \quad \text{and} \quad k_2 = k \sin \phi,$$ (12)

in which the relation (7) is still valid. In these variables, $k_1$ and $k_2$ take values in the interval $(-\infty, \infty)$, whereas $u$ takes values in the interval $(-a(k_1^2 + k_2^2), a(k_1^2 + k_2^2))$ (Eq. 11).

2.2. The Hilbert space

On the space of integrable single valued complex functions defined on $\mathbb{R}^3$, we define the scalar product of two functions $f$ and $g$ by

$$\langle f \mid g \rangle \equiv \int_{\mathbb{R}^3} f^*(\mathbf{r})g(\mathbf{r})d^3\mathbf{r}$$ (13)
and the norm
\[ ||f|| = \sqrt{\langle f | f \rangle}. \]
We work with the Hilbert space \( \mathbb{H} \equiv L^2(\mathbb{R}^3) \), which consists of the functions integrable in modulus square.

The space \( \mathbb{R}^3 \) minus the z axis, \( \tilde{\mathbb{R}}^3 \equiv \mathbb{R}^3 \setminus z \), is mapped onto a set \( \mathbb{M} \) in the \( (k, u, \phi) \) space, where \( \phi \in [0, 2\pi) \), \( k \in (0, \infty) \), and \( a \in (-a(k), a(k)) \). Then, the functions \( f(\mathbf{r}), g(\mathbf{r}) \), from \( \mathbb{H} \), are mapped into the functions \( \tilde{f}(k, u, \phi), \tilde{g}(k, u, \phi) \) defined on the set \( \mathbb{M} \). The volume element is transformed as \[33\]
\[ dx dy dz = \frac{k^3}{5mc} dk du d\phi \]
so the scalar product and the norm (Eqs 15 and 13) are
\[ \langle f | g \rangle = \langle \tilde{f} | \tilde{g} \rangle = \int_0^{2\pi} \int_0^\infty \int_{-a(k)}^{a(k)} du \tilde{f}^*(u, k, \phi) \tilde{g}(u, k, \phi) \quad \text{and} \quad ||f|| = \sqrt{\langle f | f \rangle}, \]
respectively. Then, by \( \tilde{\mathbb{H}} \equiv L^2(\mathbb{M}) \) we denote the Hilbert space of functions of finite norms defined on \( \mathbb{M} \), which is the image of \( \mathbb{H}(\mathbb{R}^3) \).

In the coordinates \( (k_1, k_2, u) \) \[12\] we have the relation
\[ dx dy dz = \frac{2k^2}{10mc} dk_1 dk_2 du, \]
\[ (f | g) = \langle \tilde{f} | \tilde{g} \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-a(\sqrt{k_1^2+k_2^2})}^{a(\sqrt{k_1^2+k_2^2})} du \tilde{f}^*(k_1, k_2, u) \tilde{g}(k_1, k_2, u) \quad \text{and} \quad ||\tilde{f}|| = \sqrt{\langle \tilde{f} | \tilde{f} \rangle}, \]
respectively. The domain of definition, \( k_1, k_2 \in (-\infty, \infty) \) and \( u \in \left(-a(\sqrt{k_1^2+k_2^2}), a(\sqrt{k_1^2+k_2^2})\right) \), \( \mathbb{M}_1 \) and the Hilbert space of functions of finite norms on \( \mathbb{M}_1 \) is denoted by \( \tilde{\mathbb{H}} = L^2(\mathbb{M}_1) \).

2.3. Boundary conditions and eigenfunctions of \( \tilde{T}_3 \)
In both sets of coordinates, \( (k, u, \phi) \) and \( (k_1, k_2, u) \), the operator \( \tilde{T}_3 \) is defined as \(-i\hbar \partial / \partial u\). The sets \( \mathbb{M} \) \( (k, u, \phi) \) and \( \mathbb{M}_1 \) \( (k_1, k_2, u) \) correspond to the whole \( \mathbb{R}^3 \) \( (x, y, z) \) space and no boundary conditions are imposed on their frontiers—that is, when \( u = \pm a(k) \) in \( (k, u, \phi) \) and \( u = \pm a(\sqrt{k_1^2+k_2^2}) \) in \( (k_1, k_2, u) \).

Then, in the coordinates \( (k, u, \phi) \), \( \tilde{T}_3 \) is defined on the set of smooth functions on \( \mathbb{M} \) and we can impose the boundary conditions \[33\]
\[ \tilde{f}[k, -a(k), \phi] = \tilde{f}[k, a(k), \phi] e^{i\theta(k, \phi)}, \]
where \( \theta(k, \phi) \) can be any function of \( k \) and \( \phi \). Of course, the same conclusion is reached working in the \( (k_1, k_2, u) \) space, where the boundary conditions read
\[ \tilde{\tilde{f}}[k_1, k_2, -a(\sqrt{k_1^2+k_2^2})] = \tilde{\tilde{f}}[k_1, k_2, a(\sqrt{k_1^2+k_2^2})] e^{i\theta(k, \phi)}. \]
A set of orthonormal eigenfunctions for the \( \hat{T}_3 \) operator in the \((k, u, \phi)\) space, which satisfy periodic boundary conditions in the \(u\) direction, was proposed in Ref. [33]:

\[
\mathcal{T}_{k_0, t_{k_0}, m}(k, u, \phi) \equiv \frac{1}{2k \sqrt{2\pi \hbar C_a}} \delta(k - k_0)e^{i tk_0 u}e^{i m\phi},
\]

where \(k_0 \in (0, \infty), t_{k_0} \equiv n \pi \hbar / a(k_0)\), whereas \(m\) and \(n\) are integers. We see that the functions (20) are localized on the \(k\) axis of the space \(\mathbb{M}\).

If \(\hat{T}_3\) is not defined on the whole space \(\mathbb{R}^3\), then different boundary conditions may be imposed. For example, the definition domain may be a finite region \(\mathbb{D}\) of \(\mathbb{R}^3\), with Dirichlet boundary conditions on the frontier (e.g. a nucleus, a region of a condensed matter system, or an element of a metamaterial).

3. Commuting set of operators

In order to find other operators that commute with \(\hat{T}_3\), we notice that in the space \((k, u, \phi)\) any operator which is a function of \(k, \partial/\partial k, \partial/\partial u,\) and \(\partial/\partial \phi\) commutes with both, \(\hat{T}_3\) and \(\hat{L}_3\). Similarly, in the space \((k_1, k_2, u)\), any operator that is a function of \(k_1, k_2, \partial/\partial k_1, \partial/\partial k_2,\) and \(\partial/\partial u\) commutes with \(\hat{T}_3\). In this section, we calculate the operators \(\partial/\partial k\) (in the \((k, u, \phi)\) space), \(\partial/\partial k_1\), and \(\partial/\partial k_2\) (in the \((k_1, k_2, u)\) space). Having these, we can form complete sets of commuting operators involving partial derivatives. For example, in the coordinates \((k_1, k_2, u)\), the operators \(\hat{p}^{(k1)} \equiv -i\hbar \partial/\partial k_1, \hat{p}^{(k2)} \equiv -i\hbar \partial/\partial k_2,\) and \(\hat{T}_3 \equiv -i\hbar \partial/\partial u\) resemble the three components of a “momentum operator” and form a complete set of commuting operators. In the coordinates \((k, u, \phi)\), the operators \(\hat{T}_3 \equiv -i\hbar \partial/\partial u\) and \(\hat{L}_3 \equiv -i\hbar \partial/\partial \phi\) correspond to the projections on the \(z\) axis of the toroidal moment and of the angular momentum, whereas the third operator, defined as \(\hat{p}^{(k)} \equiv -i\hbar \partial/\partial k\), represents the projection of the “momentum operator” in the \((k_1, k_2, u)\) coordinates, on the radial direction \(k \equiv \sqrt{k_1^2 + k_2^2}\).

3.1. The operator \(\hat{p}^{(k)}\) in the \((k, u, \phi)\) space

From Eqs. (10) we obtain

\[
\begin{align*}
du & = \frac{\partial f_u}{\partial z} dz + \frac{\partial f_u}{\partial k} dk, \quad (21a) \\
\frac{\partial f_u}{\partial z} & = \frac{-10mc}{\sqrt{z^4 + 4k^4}} \quad (22a) \\
\frac{\partial f_u}{\partial k} & = \frac{5mc}{\sqrt{t^4 + 4k^4}} \int_0^z \frac{16k^3}{(t^4 + 4k^4)^{3/2}} dt \equiv 5mc \int_0^z \frac{16 \left( \rho^2 (z^2 + \rho^2) \right)^{3/4}}{\left( t^4 + 4 \left( \rho^2 (z^2 + \rho^2) \right) \right)^{3/2}} dt \quad (22b) \\
\frac{\partial k}{\partial \rho} & = \frac{2 \rho^2 + z^2}{2 \sqrt{\rho} (\rho^2 + z^2)^{3/4}} \quad (22c) \\
\frac{\partial k}{\partial z} & = \frac{\sqrt{\rho} z}{2 (\rho^2 + z^2)^{3/4}} \quad (22d)
\end{align*}
\]
From the condition \( du = 0 \) and Eq. (21a) we obtain the derivative of \( z \) with respect to \( k \) at constant \( u \):

\[
\left. \frac{dz}{dk} \right|_{u} = -\frac{\partial f_u}{\partial k} \left( \frac{\partial f_u}{\partial z} \right)^{-1}
\]  

(23)

To obtain the derivative of \( \rho \) with respect to \( z \) at constant \( u \), we plug Eq. (23) into Eq. (21b) and, using also Eqs. (22), we obtain

\[
\left. \frac{d\rho}{dz} \right|_{u} = \left( \frac{dk}{dz} \right) \left. \frac{d\rho}{dk} \right|_{u} - \frac{\partial k}{\partial z} \frac{\partial k}{\partial \rho} \left( \frac{\partial f_u}{\partial z} \right)^{-1} - \frac{\sqrt{\frac{\rho z^2 (\rho^2 + z^2)^{3/4}}{2\rho^3 + z^2}}}{\sqrt{\rho z^2 (\rho^2 + z^2)^{3/4}}}. \]

(24)

Combining (24) with (23), we write

\[
\left. \frac{d\rho}{dk} \right|_{u} = \left( \left. \frac{d\rho}{dz} \right|_{u} \right) 
\]

(25a)

Then, the partial derivative in the \((k,u,\phi)\) space of an arbitrary function \( \tilde{F}(k,u,\phi) \equiv F(\rho,z,\phi) \) may be written in cylindrical coordinates as

\[
\frac{\partial \tilde{F}(k,u,\phi)}{\partial k} = \frac{\partial F}{\partial \rho} \left. \frac{d\rho}{dk} \right|_{u} + \frac{\partial F}{\partial z} \left. \frac{dz}{dk} \right|_{u}. \]

(25b)

Combining Eqs. (22) and (25) we obtain the expression for \( \hat{p}(k) \):

\[
\hat{p}(k) \equiv -i\hbar \frac{\partial}{\partial k} = -i\hbar \left( \left. \frac{d\rho}{dk} \right|_{u} \frac{\partial}{\partial \rho} + \left. \frac{dz}{dk} \right|_{u} \frac{\partial}{\partial z} \right). \]

(26)

On the other hand, if we invert Eqs. (10), by first formally writing from the second equation \( z \) as a function of \( k \) and \( u \) (say, \( z(k,u) \), since we do not have an analytical expression), then, from the first equation,

\[
\rho(k,u) = \frac{z(k,u)}{\sqrt{2}} \sqrt{1 + 4k^4 z^4(k,u) - 1}. \]

(27)

In these notations,

\[
\left. \frac{dz}{dk} \right|_{u} = \frac{\partial z(k,u)}{\partial k}, \quad \text{and} \quad \left. \frac{d\rho}{dk} \right|_{u} = \frac{\partial \rho(k,u)}{\partial k} = -\frac{\sqrt{1 + 4k^4 z^4(k,u) - 1}}{\sqrt{2}} \frac{1}{\sqrt{1 + 4k^4 z^4(k,u)}} \frac{\partial z}{\partial k} + \frac{2\sqrt{2k^3 z^3}}{\sqrt{1 + 4k^4 z^4(k,u) - 1}} \frac{1}{\sqrt{1 + 4k^4 z^4(k,u)}} \frac{\partial z}{\partial k}, \]

(28)

which may be plugged into (26), to obtain \( \hat{p}(k) \).

Therefore, the operator \( \hat{p}(k) = -i\hbar \frac{\partial}{\partial k} \) in the \((k,u,\phi)\) space may be expressed in terms of the \((x,y,z)\) coordinates and has the form

\[
\hat{p}(k) = -i\hbar \frac{\partial}{\partial k} = -i\hbar \left. \frac{\partial f_u}{\partial k} \right|_{u} \left( \frac{\partial f_u}{\partial z} \right)^{-1} \left[ \frac{\partial f_u}{\partial z} \frac{\partial f_u}{\partial k} \frac{\partial f_u}{\partial \rho} \frac{\partial f_u}{\partial \rho} + \partial k \frac{\partial}{\partial \rho} \frac{\partial f_u}{\partial \rho} - \frac{\partial}{\partial z} \right] \equiv \mathbf{P}(k) \cdot \hat{p}, \]

(29)

and all the partial derivatives are given in equations (22), whereas \( \hat{p} \equiv -i\hbar \nabla \) is the momentum operator in the \((x,y,z)\) coordinates.
Figure 3: The directions of the vector field $\mathbf{P}^{(k)}$ (i.e., $\mathbf{P}^{(k)} \equiv \mathbf{P}^{(k)}/P^{(k)}$) and the curves of constant $u(\rho, z)$. The vector field is tangent to the curves in every point.

The vector field $\mathbf{P}^{(k)}$ in cylindrical coordinates is

$$\mathbf{P}^{(k)} \equiv \frac{\partial f_u}{\partial k} \left( \frac{\partial f_u}{\partial z} \right)^{-1} \left[ \frac{(\partial f_u/\partial z)(\partial f_u/\partial k)^{-1} + \partial k/\partial \rho}{\partial k/\partial \rho} \right].$$

(30)

The directions of $\mathbf{P}^{(k)}$ (that is, $\mathbf{p}^{(k)} \equiv \mathbf{P}^{(k)}/P^{(k)}$) are drawn in Fig. 3, together with the curves of constant $u(\rho, z)$. These curves correspond to lines parallel to the $k$ axis in the $(k, u, \phi)$ space (fixed $u$ and $\phi$), so the vector field $\mathbf{P}^{(k)}$ is tangent to them in every point—similarly to $\mathbf{T}_3$ in Fig. 2.

Equations (8) and (29) may be joined into a system from which we can calculate the partial derivatives in the $(x, y, z)$ coordinates in terms of the partial derivatives in the $(k, u, \phi)$ coordinates:

$$\left[ \begin{array}{c} \frac{\partial}{\partial k} \\ \frac{\partial}{\partial u} \end{array} \right] \equiv \left[ \begin{array}{c} T^{(k)}_3 \end{array} \right] \left[ \begin{array}{c} \frac{\partial}{\partial \rho} \\ \frac{\partial}{\partial z} \end{array} \right],$$

(31)

where

$$\left[ T^{(k)}_3 \right] = \left[ \begin{array}{cc} \frac{\partial \rho(k, u)}{\partial k} & \frac{\partial z(k, u)}{\partial k} \\ \frac{z(k, u) \partial k}{10mc} & \frac{-\partial k}{\partial \rho} \frac{2z^2 + \rho^2}{10mc} \end{array} \right].$$

(32)

By inverting the system (31), we write $\partial/\partial \rho$ and $\partial/\partial z$ in terms of $\partial/\partial k$ and $\partial/\partial u$, in the natural set of coordinates for $T_3$.

### 3.2. The operators $\hat{p}^{(k_1)}$ and $\hat{p}^{(k_2)}$, in the $(k_1, k_2, u)$ space

If we switch from the coordinates $(k, u, \phi)$ to the coordinates $(k_1, k_2, u)$ we have

$$u \equiv -10mc \int_0^z \frac{dt}{\sqrt{t^4 + 4(k_1^2 + k_2^2)^2}} \equiv f_{u2}(z, k_1, k_2) \quad \text{and} \quad a(k) = \frac{10mc}{\sqrt{k_1^2 + k_2^2}} C_a.$$  

(33)

The coordinates $k_1 = k \cos \phi$ and $k_2 = k \sin \phi$ in terms of $x$, $y$, and $z$ are

$$k_1 = x \left[ 1 + \frac{z^2}{x^2 + y^2} \right]^{1/4} \equiv x \sqrt{\frac{\rho}{\rho}} \quad \text{and} \quad k_2 = y \left[ 1 + \frac{z^2}{x^2 + y^2} \right]^{1/4} \equiv y \sqrt{\frac{\rho}{\rho}}.$$  

(34)
Hence, we define the operators
\[ \hat{p}^{(k_1)} = -i\hbar \frac{\partial}{\partial k_1} \quad \text{and} \quad \hat{p}^{(k_2)} = -i\hbar \frac{\partial}{\partial k_2}, \] (35)
which, by definition, satisfy the commutation relations
\[ [\hat{T}_3, \hat{p}^{(k_1)}] = [\hat{T}_3, \hat{p}^{(k_2)}] = [\hat{p}^{(k_1)}, \hat{p}^{(k_2)}] = 0 \] (36)
From Eqs. (33) and (34) we write
\[ du = \frac{\partial f_{u_2}}{\partial z} dz + \frac{\partial f_{u_2}}{\partial k_1} dk_1 + \frac{\partial f_{u_2}}{\partial k_2} dk_2, \] (37a)
\[ dk_1 = \frac{\partial k_1}{\partial x} dx + \frac{\partial k_1}{\partial y} dy + \frac{\partial k_1}{\partial z} dz, \] (37b)
\[ dk_2 = \frac{\partial k_2}{\partial x} dx + \frac{\partial k_2}{\partial y} dy + \frac{\partial k_2}{\partial z} dz, \] (37c)
where
\[ \frac{\partial f_{u_2}}{\partial z} = -10mc \sqrt{z^4 + 4(k_1^2 + k_2^2)^2}, \] (38a)
\[ \frac{\partial f_{u_2}}{\partial k_1} = 80mc (k_1^2 + k_2^2) k_1 \int_0^z dt \left[ t^4 + 4 \left( k_1^2 + k_2^2 \right)^2 \right]^{3/2}, \] (38b)
\[ \frac{\partial f_{u_2}}{\partial k_2} = 80mc (k_1^2 + k_2^2) k_2 \int_0^z dt \left[ t^4 + 4 \left( k_1^2 + k_2^2 \right)^2 \right]^{3/2}, \] (38c)
\[ \frac{\partial k_1}{\partial x} = \frac{4x^2y^2 + x^2z^2 + 2y^2z^2 + 2x^4 + 2y^4}{2(x^2 + y^2)^{5/4}(x^2 + y^2 + z^2)^{3/4}}, \] (38d)
\[ \frac{\partial k_1}{\partial y} = \frac{xyz}{2(x^2 + y^2)^{5/4}(x^2 + y^2 + z^2)^{3/4}}, \] (38e)
\[ \frac{\partial k_1}{\partial z} = \frac{xz}{2(x^2 + y^2)^{1/4}(x^2 + y^2 + z^2)^{3/4}}, \] (38f)
\[ \frac{\partial k_2}{\partial x} = \frac{2x^2y^2 + 2x^2z^2 + y^2z^2 + 2x^4 + 2y^4}{2(x^2 + y^2)^{5/4}(x^2 + y^2 + z^2)^{3/4}}, \] (38g)
\[ \frac{\partial k_2}{\partial y} = \frac{yz}{2(x^2 + y^2)^{1/4}(x^2 + y^2 + z^2)^{3/4}}, \] (38h)
\[ \frac{\partial k_2}{\partial z} = \frac{y^2}{2(x^2 + y^2)^{1/4}(x^2 + y^2 + z^2)^{3/4}}. \] (38i)

To express \( \partial / \partial k_1 \) in the \((x, y, z)\) coordinates, we impose \( du = dk_2 = 0 \) in Eq. (37a) and obtain
\[ dz = -\frac{\partial f_{u_2}}{\partial k_1} \left( \frac{\partial f_{u_2}}{\partial z} \right)^{-1} dk_1. \] (39)
Plugging (39) into (37b) we obtain
\[ -\left[ \frac{\partial f_{u_2}}{\partial z} \left( \frac{\partial f_{u_2}}{\partial k_1} \right)^{-1} + \frac{\partial k_1}{\partial z} \right] dz = \frac{\partial k_1}{\partial x} dx + \frac{\partial k_1}{\partial y} dy, \] (40)
whereas from (37c) and $dk_2 = 0$ we obtain

$$dy = - \left( \frac{\partial k_2}{\partial y} \right)^{-1} \left( \frac{\partial k_2}{\partial x} dx + \frac{\partial k_2}{\partial z} dz \right).$$

(41)

Plugging (41) into (40) we obtain an equation in $dx$ and $dz$,

$$dx = \frac{\partial k_1}{\partial y} \frac{\partial k_2}{\partial z} \left( \frac{\partial k_2}{\partial y} \right)^{-1} - \frac{\partial f_{u_2}}{\partial z} \left( \frac{\partial f_{u_2}}{\partial k_1} \right)^{-1} - \frac{\partial k_1}{\partial z} d\zeta.$$

(42)

Plugging (42) into (41) we obtain

$$dy = - \left( \frac{\partial k_2}{\partial y} \right)^{-1} \left[ \frac{\partial k_1}{\partial y} \frac{\partial k_2}{\partial z} \left( \frac{\partial k_2}{\partial y} \right)^{-1} - \frac{\partial f_{u_2}}{\partial z} \left( \frac{\partial f_{u_2}}{\partial k_1} \right)^{-1} - \frac{\partial k_1}{\partial z} \right] dz.$$

(43)

Equations (39), (42), and (43) give us the derivatives at constant $u$ and $k_2$:

$$\frac{dz}{dk_1} \bigg|_{u,k_2} = -\frac{\partial f_{u_2}}{\partial k_1} \left( \frac{\partial f_{u_2}}{\partial z} \right)^{-1}, \quad \frac{dx}{dz} \bigg|_{u,k_2} = \frac{\partial k_1}{\partial y} \frac{\partial k_2}{\partial z} \left( \frac{\partial k_2}{\partial y} \right)^{-1} - \frac{\partial f_{u_2}}{\partial z} \left( \frac{\partial f_{u_2}}{\partial k_1} \right)^{-1} - \frac{\partial k_1}{\partial z},$$

and

$$\frac{dy}{dz} \bigg|_{u,k_2} = - \left( \frac{\partial k_2}{\partial y} \right)^{-1} \left[ \frac{\partial k_1}{\partial y} \frac{\partial k_2}{\partial z} \left( \frac{\partial k_2}{\partial y} \right)^{-1} - \frac{\partial f_{u_2}}{\partial z} \left( \frac{\partial f_{u_2}}{\partial k_1} \right)^{-1} - \frac{\partial k_1}{\partial z} \right] dz.$$

(44)

Finally, from (44) we obtain the expression for $\hat{p}^{(k_1)}$

$$\hat{p}^{(k_1)} \equiv -ih \frac{\partial}{\partial k_1} = -ih \frac{dz}{dk_1} \bigg|_{u,k_2} \left\{ \frac{dx}{dz} \bigg|_{u,k_2} \frac{\partial}{\partial x} + \frac{dy}{dz} \bigg|_{u,k_2} \frac{\partial}{\partial y} + \frac{\partial}{\partial z} \right\}.$$

(45)

Similarly, we can obtain the expression for $\hat{p}^{(k_2)}$. From Eq. (37a), with the conditions $du = dk_1 = 0$, we get

$$dz = -\frac{\partial f_{u_2}}{\partial k_2} \left( \frac{\partial f_{u_2}}{\partial z} \right)^{-1} dk_2.$$

(46)

Plugging (46) into (37c) we obtain

$$\left[ \frac{\partial f_{u_2}}{\partial z} \left( \frac{\partial f_{u_2}}{\partial k_2} \right)^{-1} + \frac{\partial k_2}{\partial z} \right] dz = \frac{\partial k_1}{\partial x} dx + \frac{\partial k_1}{\partial y} dy,$$

(47)

whereas from (37b) and $dk_1 = 0$ we have

$$dy = - \left( \frac{\partial k_1}{\partial y} \right)^{-1} \left( \frac{\partial k_1}{\partial x} dx + \frac{\partial k_1}{\partial z} dz \right).$$

(48)

Plugging (48) into (47) we obtain

$$dx = \frac{\partial k_2}{\partial y} \frac{\partial k_1}{\partial z} \left( \frac{\partial k_1}{\partial y} \right)^{-1} - \frac{\partial f_{u_2}}{\partial z} \left( \frac{\partial f_{u_2}}{\partial k_2} \right)^{-1} - \frac{\partial k_2}{\partial z} d\zeta.$$

(49)
Plugging (49) into (48) we obtain
\[
dy = - \left( \frac{\partial k_1}{\partial y} \right)^{-1} \left[ \frac{\partial k_1}{\partial x} \frac{\partial k_1}{\partial y} \frac{\partial k_1}{\partial z} \left( \frac{\partial f_{u_2}}{\partial k_2} \right)^{-1} - \frac{\partial f_{u_2}}{\partial z} \left( \frac{\partial f_{u_2}}{\partial k_2} \right)^{-1} - \frac{\partial k_1}{\partial z} \right] dz \tag{50}
\]

From Eqs. (46), (49), and (50) we obtain
\[
\frac{dz}{dk_2} \bigg|_{u,k_1} = - \frac{\partial f_{u_2}}{\partial k_2} \left( \frac{\partial f_{u_2}}{\partial z} \right)^{-1}, \quad \frac{dx}{dz} \bigg|_{u,k_1} = \frac{\partial k_2}{\partial x} \frac{\partial k_1}{\partial y} \frac{\partial k_1}{\partial z} \left( \frac{\partial f_{u_2}}{\partial k_2} \right)^{-1} - \frac{\partial f_{u_2}}{\partial z} \left( \frac{\partial f_{u_2}}{\partial k_2} \right)^{-1} - \frac{\partial k_2}{\partial z},
\]

so
\[
\hat{p}^{(k_2)} = -i\hbar \frac{\partial}{\partial k_2} = -i\hbar \frac{dz}{dk_2} \bigg|_{u,k_1} \left\{ \frac{dx}{dz} \bigg|_{u,k_1} \frac{\partial}{\partial x} + \frac{dy}{dz} \bigg|_{u,k_1} \frac{\partial}{\partial y} + \frac{\partial}{\partial z} \right\}. \tag{52}
\]

If we formally invert Eqs. (33) to write \( z \) as a function of \( k_1, k_2, \) and \( u \), then, from Eqs. (34) we obtain
\[
x(k_1, k_2, u) = f_x[k_1, k_2, z(k_1, k_2, u)] \quad \text{and} \quad y(k_1, k_2, u) = f_y[k_1, k_2, z(k_1, k_2, u)], \tag{53a}
\]

where
\[
f_x(k_1, k_2, z) = \frac{k_1 z}{\sqrt{k_1^2 + k_2^2}} \sqrt{1 + 4 \left( \frac{k_1^2 + k_2^2}{z^2} \right)} - 1 \quad \text{and} \quad f_y(k_1, k_2, z) = \frac{k_2 z}{\sqrt{k_1^2 + k_2^2}} \sqrt{1 + 4 \left( \frac{k_1^2 + k_2^2}{z^2} \right)} - 1. \tag{53b}
\]

From the definition of \( z(k_1, k_2, u) \), we write formally,
\[
\frac{dz}{dk_1} \bigg|_{u,k_2} = \frac{\partial z(k_1, k_2, u)}{\partial k_1}, \quad \frac{dz}{dk_2} \bigg|_{u,k_1} = \frac{\partial z(k_1, k_2, u)}{\partial k_2}. \tag{54}
\]
whereas the other derivatives are

\[
\begin{align*}
\frac{\partial f_x(k_1, k_2, z)}{\partial k_1} &= \frac{k_2^2 z}{(k_1^2 + k_2^2)^{3/2}} - \sqrt{1 + \frac{4(k_1^2 + k_2^2)^2}{z^4}} + 1 + 4 \left(\frac{k_1^2 + k_2^2}{k_1^2 z^4}\right)^2, \\
\frac{\partial f_x(k_1, k_2, z)}{\partial k_2} &= \frac{k_1 k_2 z}{(k_1^2 + k_2^2)^{3/2}} \sqrt{1 + \frac{4(k_1^2 + k_2^2)^2}{z^4}} - 1, \\
\frac{\partial f_x(k_1, k_2, z)}{\partial z} &= -\frac{k_1}{\sqrt{k_1^2 + k_2^2}} \left[ 1 - \frac{1}{\sqrt{1 + \frac{4(k_1^2 + k_2^2)^2}{z^4}}} \right], \\
\frac{\partial f_y(k_1, k_2, z)}{\partial k_1} &= \frac{k_1 k_2 z}{(k_1^2 + k_2^2)^{3/2}} \sqrt{1 + \frac{4(k_1^2 + k_2^2)^2}{z^4}} - 1, \\
\frac{\partial f_y(k_1, k_2, z)}{\partial k_2} &= \frac{k_2^2 z}{(k_1^2 + k_2^2)^{3/2}} \sqrt{1 + \frac{4(k_1^2 + k_2^2)^2}{z^4}} + 1 + 4 \left(\frac{k_1^2 + k_2^2}{k_1^2 z^4}\right)^2, \\
\frac{\partial f_y(k_1, k_2, z)}{\partial z} &= \frac{k_2}{\sqrt{k_1^2 + k_2^2}} \left[ 1 - \frac{1}{\sqrt{1 + \frac{4(k_1^2 + k_2^2)^2}{z^4}}} \right].
\end{align*}
\]

Plugging Eqs. (53)-(55) into the expressions for \( \hat{p}^{(k_1)} \) and \( \hat{p}^{(k_2)} \), we obtain

\[
\hat{p}^{(k_1)} = -i\hbar \frac{\partial}{\partial k_1} = -i\hbar \left\{ \frac{\partial x(k_1, k_2, u)}{\partial k_1} \frac{\partial}{\partial x} + \frac{\partial y(k_1, k_2, u)}{\partial k_1} \frac{\partial}{\partial y} + \frac{\partial z(k_1, k_2, u)}{\partial k_1} \frac{\partial}{\partial z} \right\}
- i\hbar \left\{ \frac{\partial f_x(k_1, k_2, z)}{\partial k_1} \frac{\partial}{\partial x} + \frac{\partial f_x(k_1, k_2, z)}{\partial k_2} \frac{\partial}{\partial y} + \frac{\partial f_x(k_1, k_2, z)}{\partial z} \frac{\partial}{\partial z} \right\}
\]

\[
+ \left[ \frac{\partial f_y(k_1, k_2, z)}{\partial k_1} \frac{\partial}{\partial x} + \frac{\partial f_y(k_1, k_2, z)}{\partial k_2} \frac{\partial}{\partial y} + \frac{\partial f_y(k_1, k_2, z)}{\partial z} \frac{\partial}{\partial z} \right].
\]

and

\[
\hat{p}^{(k_2)} = -i\hbar \frac{\partial}{\partial k_2} = -i\hbar \left\{ \frac{\partial x(k_1, k_2, u)}{\partial k_2} \frac{\partial}{\partial x} + \frac{\partial y(k_1, k_2, u)}{\partial k_2} \frac{\partial}{\partial y} + \frac{\partial z(k_1, k_2, u)}{\partial k_2} \frac{\partial}{\partial z} \right\}
- i\hbar \left\{ \frac{\partial f_x(k_1, k_2, z)}{\partial k_2} \frac{\partial}{\partial x} + \frac{\partial f_x(k_1, k_2, z)}{\partial k_2} \frac{\partial}{\partial y} + \frac{\partial f_x(k_1, k_2, z)}{\partial z} \frac{\partial}{\partial z} \right\}
\]

\[
+ \left[ \frac{\partial f_y(k_1, k_2, z)}{\partial k_2} \frac{\partial}{\partial x} + \frac{\partial f_y(k_1, k_2, z)}{\partial k_2} \frac{\partial}{\partial y} + \frac{\partial f_y(k_1, k_2, z)}{\partial z} \frac{\partial}{\partial z} \right].
\]
Therefore, the operators \( \hat{p}^{(k1)} \) and \( \hat{p}^{(k2)} \) in the \((x, y, z)\) coordinates have the expressions:

\[
\hat{p}^{(k1)} = -i\hbar \frac{\partial}{\partial k_1} = -i\hbar \frac{\partial f_{x2}}{\partial k_1} \left( \frac{\partial f_{x2}}{\partial z} \right)^{-1} \left\{ \frac{\partial f_{x2}}{\partial y} \frac{\partial f_{x2}}{\partial z} - \frac{\partial f_{x2}}{\partial z} \frac{\partial f_{x2}}{\partial y} \right\}^{-1} \frac{\partial f_{x2}}{\partial x} - \frac{\partial f_{x2}}{\partial x} \frac{\partial f_{x2}}{\partial z} \left( \frac{\partial f_{x2}}{\partial y} \right)^{-1} \frac{\partial f_{x2}}{\partial y} - \frac{\partial f_{x2}}{\partial y} \frac{\partial f_{x2}}{\partial z} \left( \frac{\partial f_{x2}}{\partial x} \right)^{-1} \frac{\partial f_{x2}}{\partial x} - \frac{\partial f_{x2}}{\partial x} \frac{\partial f_{x2}}{\partial z} \left( \frac{\partial f_{x2}}{\partial y} \right)^{-1} \frac{\partial f_{x2}}{\partial y} - \frac{\partial f_{x2}}{\partial y} \frac{\partial f_{x2}}{\partial z} \left( \frac{\partial f_{x2}}{\partial x} \right)^{-1} \frac{\partial f_{x2}}{\partial x} - \frac{\partial f_{x2}}{\partial z} \left( \frac{\partial f_{x2}}{\partial y} \right)^{-1} \frac{\partial f_{x2}}{\partial y} - \frac{\partial f_{x2}}{\partial y} \frac{\partial f_{x2}}{\partial z} \left( \frac{\partial f_{x2}}{\partial x} \right)^{-1} \frac{\partial f_{x2}}{\partial x} - \frac{\partial f_{x2}}{\partial x} \frac{\partial f_{x2}}{\partial z} \left( \frac{\partial f_{x2}}{\partial y} \right)^{-1}
\]

\[
\hat{p}^{(k2)} = -i\hbar \frac{\partial f_{x2}}{\partial k_2} \left( \frac{\partial f_{x2}}{\partial z} \right)^{-1} \left\{ \frac{\partial f_{x2}}{\partial y} \frac{\partial f_{x2}}{\partial z} - \frac{\partial f_{x2}}{\partial z} \frac{\partial f_{x2}}{\partial y} \right\}^{-1} \frac{\partial f_{x2}}{\partial x} - \frac{\partial f_{x2}}{\partial x} \frac{\partial f_{x2}}{\partial z} \left( \frac{\partial f_{x2}}{\partial y} \right)^{-1} \frac{\partial f_{x2}}{\partial y} - \frac{\partial f_{x2}}{\partial y} \frac{\partial f_{x2}}{\partial z} \left( \frac{\partial f_{x2}}{\partial x} \right)^{-1} \frac{\partial f_{x2}}{\partial x} - \frac{\partial f_{x2}}{\partial x} \frac{\partial f_{x2}}{\partial z} \left( \frac{\partial f_{x2}}{\partial y} \right)^{-1} \frac{\partial f_{x2}}{\partial y} - \frac{\partial f_{x2}}{\partial y} \frac{\partial f_{x2}}{\partial z} \left( \frac{\partial f_{x2}}{\partial x} \right)^{-1} \frac{\partial f_{x2}}{\partial x} - \frac{\partial f_{x2}}{\partial z} \left( \frac{\partial f_{x2}}{\partial y} \right)^{-1} \frac{\partial f_{x2}}{\partial y} - \frac{\partial f_{x2}}{\partial y} \frac{\partial f_{x2}}{\partial z} \left( \frac{\partial f_{x2}}{\partial x} \right)^{-1} \frac{\partial f_{x2}}{\partial x} - \frac{\partial f_{x2}}{\partial x} \frac{\partial f_{x2}}{\partial z} \left( \frac{\partial f_{x2}}{\partial y} \right)^{-1} \frac{\partial f_{x2}}{\partial y} - \frac{\partial f_{x2}}{\partial y} \frac{\partial f_{x2}}{\partial z} \left( \frac{\partial f_{x2}}{\partial x} \right)^{-1} \frac{\partial f_{x2}}{\partial x} - \frac{\partial f_{x2}}{\partial x} \frac{\partial f_{x2}}{\partial z} \left( \frac{\partial f_{x2}}{\partial y} \right)^{-1}
\]

The operators \( \hat{p}^{(k1)}, \hat{p}^{(k2)}, \hat{T}_3 \) form a CSOC. In the \((k_1, k_2, u)\) space, the eigenfunctions corresponding to the \( \hat{p}^{(k1)}, \hat{p}^{(k2)}, \) and \( \hat{T}_3 \) observables are planewaves denoted in the ket notations by \( |p^{(k1)}, p^{(k2)}, t_3\rangle \), where \( \langle p^{(k1)}, p^{(k2)}, t_3 \rangle \) are the eigenvalues. On the other hand, as in Section 3.1, we can form a system of equations, using Eqs. (5) and (57):

\[
\begin{bmatrix}
\hat{p}^{(k1)} \\
\hat{p}^{(k2)} \\
\hat{T}_3
\end{bmatrix} =
\begin{bmatrix}
T_{3(k_1,k_2)}
\end{bmatrix}
\begin{bmatrix}
p_1 \\
p_2 \\
p_3
\end{bmatrix},
\text{ where } \begin{bmatrix} T_{3(k_1,k_2)} \end{bmatrix} \equiv \begin{bmatrix} (P^{(k1)})^t \\
(P^{(k2)})^t \\
(T_3^{(x,y,z)})^t
\end{bmatrix}.
\] (58)

\((\cdot)^t\) denotes the transposed of a vector or a matrix, and which may be inverted, to obtain all the components of the momentum operator \( \hat{p} \) in terms of \( \hat{p}^{(k1)}, \hat{p}^{(k2)}, \hat{T}_3 \) and \((k_1, k_2, u)\). In terms of the variables \((k_1, k_2, u)\), the vectors that appear in Eq. (58) are (see Eqs. 5 and 53-56):

\[
P^{(k1)} = \begin{bmatrix}
\frac{\partial f_{x2}(k_1, k_2, z)}{\partial k_1} + \frac{\partial f_{x2}(k_1, k_2, z)}{\partial z} \frac{\partial z(k_1, k_2, u)}{\partial k_1} \\
\frac{\partial f_{x2}(k_1, k_2, z)}{\partial k_2} + \frac{\partial f_{x2}(k_1, k_2, z)}{\partial z} \frac{\partial z(k_1, k_2, u)}{\partial k_2}
\end{bmatrix},
\] (59a)

\[
P^{(k2)} = \begin{bmatrix}
\frac{\partial f_{x2}(k_1, k_2, z)}{\partial k_1} + \frac{\partial f_{x2}(k_1, k_2, z)}{\partial z} \frac{\partial z(k_1, k_2, u)}{\partial k_1} \\
\frac{\partial f_{x2}(k_1, k_2, z)}{\partial k_2} + \frac{\partial f_{x2}(k_1, k_2, z)}{\partial z} \frac{\partial z(k_1, k_2, u)}{\partial k_2}
\end{bmatrix},
\] (59b)

\[
T_3^{(x,y,z)} = \frac{1}{10mc} \begin{bmatrix}
x(k_1, k_2, u)z(k_1, k_2, u) \\
y(k_1, k_2, u)z(k_1, k_2, u) \\
z^2(k_1, k_2, u) - 2r^2(k_1, k_2, u)
\end{bmatrix},
\] (59c)

4. Conclusions

We analyzed the quantum properties of the toroidal dipole operator, by studying its projection \( \hat{T}_3 \) on the \( z \) axis. For this, we changed from the cylindrical and Cartesian coordinates to what we called the “natural coordinates” of the operator, \((k, u, \phi)\) and \((k_1, k_2, u)\), respectively, where \(k_1 = k \cos \phi\) and \(k_2 = k \sin \phi\). The advantage of the natural coordinates is that \( \hat{T}_3 \) gets the much simpler form \( \hat{T}_3 = -i\hbar \partial / \partial u \) and some of its properties become more apparent. For example, in the coordinates \((k, u, \phi)\) and \((k_1, k_2, u)\), the variable \( u \) takes values in a finite interval \((-a(k), a(k))\) for any finite value of \( k \equiv \sqrt{k_1^2 + k_2^2} \), where \( a(k) = 10mcC_a/k \) (Eq. 11). This property ensures the integrability of the modulus square of the wavefunctions without the necessity to impose zero boundary condition on the border, which implies that \( \hat{T}_3 \) (as well as all the other projections of the toroidal dipole operator) is hypermaximal.
We used the natural coordinates also to find operators that commute with $\hat{T}_3$. For example, any operator that is a function of $k$, $\partial/\partial k$, $\partial/\partial u$, and $\partial/\partial \phi$ commutes with both, $\hat{T}_3$ and $\hat{L}_3$, whereas any operator that is a function of $k_1$, $k_2$, $\partial/\partial k_1$, $\partial/\partial k_2$, and $\partial/\partial u$ commutes with $\hat{T}_3$. Therefore, we constructed the operators $\hat{p}^{(k)} \equiv -i\hbar \partial/\partial k$, $\hat{p}^{(k_1)} \equiv -i\hbar \partial/\partial k_1$, and $\hat{p}^{(k_2)} \equiv -i\hbar \partial/\partial k_2$, which all commute with $\hat{T}_3$ and form two sets of commuting operators, $(\hat{p}^{(k)}, \hat{T}_3, \hat{L}_3)$ and $(\hat{p}^{(k_1)}, \hat{p}^{(k_2)}, \hat{T}_3)$, where $\hat{L}_3$ is the projection of the angular momentum operator on the $z$ axis.

We also briefly discussed the eigenfunctions and eigenvectors of $\hat{T}_3$, noticing that in physical systems (in nuclear physics [1, 31, 6], solid state physics [34], and metamaterials [25, 26, 32]) toroidal moments are not generated by currents corresponding to these eigenfunctions, that is, currents along the continuous lines in Fig. 2(a), but they are associated, in general, with current distributions along the poloidal lines of tori, as depicted in Fig. 1. Therefore, one can use the sets of commuting operators introduced here to construct new operators acting on closed lines of currents, which are more appropriate for physical (finite) systems, are self-adjoint, and correspond to observables. Such operators may be used to identify physical systems or design metamaterials in which their eigenfunctions (which are also eigenfunctions of $\hat{T}_3$) may be formed, eventually with quantized eigenvalues. The observation of the quantization of the toroidal momentum eigenvalues would constitute a signature for the toroidal properties of a system as well as an indication for its quantum properties. This subject will be analyzed elsewhere.

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