

Unveiling the quantum toroidal dipole

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The electromagnetic response of matter is governed by three fundamental multipole families: electric, magnetic, and toroidal. While the electric and magnetic are cornerstones of physics, the toroidal dipole (TD) has eluded direct, quantitative measurement for over 60 yr. Its far-field signature is masked by the electric dipole, and its behavior in the quantum regime remains largely unexplored. We address this long-standing problem by presenting a complete quantum-mechanical formalism for the TD in a nanostructure and proposing a spectroscopic method for its direct measurement. Focusing on a particle confined to a toroidal manifold—a geometry physically realized in systems such as carbon nanotube tori and topological insulator nanorings—we analyze the spectral response to an external toroidal current. We demonstrate that the resulting Aharonov-Bohm-like energy shifts are directly proportional to the expectation value of the TD operator. The transition energies exhibit a linear dependence on this current, with a quantized slope that directly reveals the change in the TD quantum number between eigenstates. This provides a clear experimental blueprint to unveil, measure, and characterize this elusive third multipole moment and its quantum nature, opening avenues in quantum metamaterials, nanoscience, and the study of fundamental symmetries.

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I. INTRODUCTION

The interaction between matter and electromagnetic fields is fundamentally described by the multipole expansion of charge-current distributions. For over a century, physics and technology have been built on the foundation of two multipole families: the electric and the magnetic. However, a third, independent multipole family—the toroidal—is required for a complete description of electromagnetism. First conceptualized by Zel'dovich in 1957 as the anapole, a parity-violating static moment in nuclear weak interactions [1], the concept was generalized by Dubovik and Cheshkov into a full, dynamic multipole family, distinct in its symmetries from its electric and magnetic counterparts [2,3].

Despite their fundamental nature, toroidal moments have remained one of the most elusive quantities in physics. Their primary challenge is that their far-field radiation pattern is identical to that of an electric dipole, effectively masking their distinct contribution in conventional scattering and emission experiments. This has spurred decades of effort to find

indirect evidence of their existence across all scales. In nuclear physics, the toroidal moment has been identified as a key component of low-energy $E1$ modes and pygmy dipole resonances [4,5], while the related static anapole moment was famously measured in atomic cesium [6]. In solid-state physics and metamaterials, the field has seen a resurgence in exploring toroidal order in multiferroics and, most notably, in nanostructured metamaterials designed to exhibit strong toroidal responses [7,8].

This progress, however, faces two profound limitations. First, existing evidence for toroidal dipoles (TDs) is almost entirely *indirect*. It relies on measuring far-field scattering or absorption and fitting these data to simulations that *assume* a toroidal current distribution. A direct, quantitative measurement of the toroidal dipole moment itself has never been achieved. Second, the vast majority of studies in metamaterials and nanosystems treat the toroidal dipole *classically*. As these systems shrink to the nanoscale, a full quantum-mechanical formalism is essential. The toroidal dipole, as a quantum-mechanical quantity, has not been rigorously explored, nor has its potential quantization been observed.

This paper bridges this fundamental gap. We provide a complete quantum-mechanical formalism for the toroidal dipole in a nanoscale system. Building on our previous work, which established the toroidal dipole operator as a self-adjoint (Hermitian) operator and thus a true quantum observable [9–11], we now propose a method for its *direct* and *quantitative* measurement. We analyze a canonical quantum system—a particle on a toroidal manifold—and show

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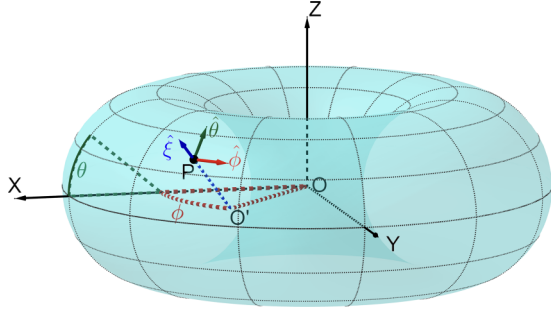


FIG. 1. The system consists of a particle of charge q and mass m_p on a thin layer between two tori. Both these tori have the same center O , rotation axis z , and major radii R , but they have different minor radii, r and $r + \xi_{\max}$, such that $r + \xi_{\max} < R$ and $\xi_{\max} \ll r$. The system is described in the orthogonal curvilinear coordinates θ, ϕ, ξ , where $\phi \in [0, 2\pi)$ is the azimuthal angle, $\theta \in [0, 2\pi)$ is the angle between the minor and the major radii, and $\xi \in [0, \xi_{\max}]$ is the coordinate that runs along the minor radius. The unit vectors of the local coordinates system are $\hat{\theta}, \hat{\phi}, \hat{\xi}$. A straight filiform current I of length L runs along the z axis, symmetrically with respect to the (xy) plane. We assume that $L \gg R$ and the circuit is closed in such a way that only the straight portion L significantly influences the particle.

that its energy levels shift in response to an external current (via the Aharonov-Bohm effect). This geometry finds direct experimental realization in diverse nanoscopic systems, ranging from self-assembled semiconductor quantum rings [12,13] and single-walled carbon nanotube tori [14,15] to bent core-shell nanowires [16] and topological insulator (TI) nanorings [17]. We prove that the resulting spectroscopic energy shift is directly proportional to the expectation value of the toroidal dipole operator. This establishes a clear experimental blueprint to measure the toroidal moment by observing transition energies. Furthermore, we show that the change in the toroidal moment between eigenstates is quantized, a prediction that can now be experimentally verified.

The remainder of this paper is organized as follows. In Sec. II, we present the complete theoretical framework, deriving the quantum-mechanical Hamiltonian and the toroidal dipole operator for a particle confined to a toroidal manifold, and establishing the Aharonov-Bohm periodicity of the system. In Sec. III, we present our main numerical results, solving the eigenvalue problem to find the complete energy spectrum and the toroidal dipole expectation values, and we analyze the direct link between the energy spectrum and the toroidal moment. Finally, in Sec. IV, we summarize our findings and discuss their direct experimental implications for a class of spectroscopic measurements.

II. THEORETICAL FRAMEWORK

We consider a quantum particle of mass m_p and charge q confined to a thin toroidal membrane of major radius R and minor (interior) radius r , as depicted in Fig. 1. The system is described in a set of orthogonal curvilinear coordinates (θ, ϕ, ξ) , where $\theta, \phi \in [0, 2\pi)$ are the poloidal and azimuthal angles, respectively, and $\xi \in [0, \xi_{\max}]$ is the radial coordinate along the minor radius. The particle's wavefunctions $\psi(\theta, \phi, \xi)$ belong to the Hilbert space of square-integrable

functions and obey the boundary conditions:

$$\begin{aligned} \psi(\theta, \phi, \xi) &= \psi(\theta + 2\pi, \phi, \xi) = \psi(\theta, \phi + 2\pi, \xi) \\ \text{and } \psi(\theta, \phi, 0) &= \psi(\theta, \phi, \xi_{\max}) = 0. \end{aligned} \quad (1)$$

To simplify the expressions throughout our analysis, we introduce a set of dimensionless quantities. Geometric parameters are scaled by the major radius R , such that $\alpha \equiv r/R \equiv 1/a$ (the inverse aspect ratio), $\alpha_\xi \equiv \xi/R$, and $\alpha_{\xi_{\max}} \equiv \xi_{\max}/R$. Operators are also made dimensionless, denoted by a tilde, by factoring out characteristic physical scales.

A. The Hamiltonian

With zero electrostatic potential, the system's Hamiltonian is given by the kinetic energy term, which includes coupling to a magnetic vector potential $\mathbf{A}$:

$$\hat{\mathcal{H}} = \frac{1}{2m_p} (\hat{\mathbf{p}} - q\mathbf{A})^2. \quad (2)$$

The canonical and kinetic momentum operators are $\hat{\mathbf{p}}_{\text{free}} = -i\hbar\nabla$ and $\hat{\mathbf{p}} = \hat{\mathbf{p}}_{\text{free}} - q\mathbf{A}$, respectively. We define dimensionless operators via $\tilde{\mathbf{p}}_{\text{free}} \equiv (R/\hbar)\hat{\mathbf{p}}_{\text{free}}$, $\tilde{\mathbf{p}} \equiv (R/\hbar)\hat{\mathbf{p}}$, $\tilde{\mathcal{H}} = (2m_p R^2/\hbar^2)\hat{\mathcal{H}}$, and $\tilde{\mathbf{A}} \equiv (qR/\hbar)\mathbf{A}$. The Hamiltonian can be decomposed into a field-free part $\tilde{\mathcal{H}}_{\text{free}}$ and a field-dependent part $\tilde{\mathcal{H}}_{\mathbf{A}}$. Furthermore, due to the geometry of the system, it is physically insightful to separate the dynamics into a two-dimensional (2D) component (involving θ and ϕ) and a transverse component (involving ξ):

$$\tilde{\mathcal{H}} = \tilde{\mathcal{H}}^{(2D)} + \tilde{\mathcal{H}}^{(\xi)}. \quad (3a)$$

The 2D Hamiltonian governing the motion on a toroidal surface is defined as

$$\tilde{\mathcal{H}}^{(2D)} \equiv \tilde{\mathcal{H}}_{\text{free}}^{(2D)} + \tilde{\mathcal{H}}_{\mathbf{A}}^{(2D)}, \quad (3b)$$

while the transverse Hamiltonian is

$$\tilde{\mathcal{H}}^{(\xi)} \equiv \tilde{\mathcal{H}}_{\text{free}}^{(\xi)} + \tilde{\mathcal{H}}_{\mathbf{A}}^{(\xi)}. \quad (3c)$$

The term $\tilde{\mathcal{H}}_{\mathbf{A}}$ has a linear $\tilde{\mathcal{H}}_{\mathbf{A},1}$ and quadratic component $\tilde{\mathcal{H}}_{\mathbf{A},2}$:

$$\begin{aligned} \tilde{\mathcal{H}}_{\mathbf{A}} &\equiv \tilde{\mathcal{H}}_{\mathbf{A},1} + \tilde{\mathcal{H}}_{\mathbf{A},2}, \text{ with } \tilde{\mathcal{H}}_{\mathbf{A},1} = \tilde{\mathcal{H}}_{\mathbf{A},1}^{(2D)} + \tilde{\mathcal{H}}_{\mathbf{A},1}^{(\xi)} \text{ and} \\ \tilde{\mathcal{H}}_{\mathbf{A},2} &= \tilde{\mathcal{H}}_{\mathbf{A},2}^{(2D)} + \tilde{\mathcal{H}}_{\mathbf{A},2}^{(\xi)}. \end{aligned} \quad (3d)$$

Consistency requires that

$$\begin{aligned} \tilde{\mathcal{H}}_{\text{free}} &= \tilde{\mathcal{H}}_{\text{free}}^{(2D)} + \tilde{\mathcal{H}}_{\text{free}}^{(\xi)}, \quad \tilde{\mathcal{H}}_{\mathbf{A}} = \tilde{\mathcal{H}}_{\mathbf{A}}^{(2D)} + \tilde{\mathcal{H}}_{\mathbf{A}}^{(\xi)}, \quad \tilde{\mathcal{H}}_{\mathbf{A}}^{(2D)} \\ &= \tilde{\mathcal{H}}_{\mathbf{A},1}^{(2D)} + \tilde{\mathcal{H}}_{\mathbf{A},2}^{(2D)}, \quad \text{and} \quad \tilde{\mathcal{H}}_{\mathbf{A}}^{(\xi)} = \tilde{\mathcal{H}}_{\mathbf{A},1}^{(\xi)} + \tilde{\mathcal{H}}_{\mathbf{A},2}^{(\xi)}. \end{aligned} \quad (3e)$$

The explicit differential forms of the momentum operators and the detailed expansion of these Hamiltonian terms in toroidal coordinates are provided in Appendix A 1.

B. The toroidal dipole operator

The second key operator for our analysis is the TD. Its projection onto the z axis is defined in Cartesian coordinates as

$$\hat{T}_3 \equiv \frac{1}{10m_p} \sum_{j=1}^3 (zx_j - 2r^2\delta_{3j})(\hat{p}_j - qA_j) \equiv \frac{\hbar R}{10m_p} \tilde{T}_3, \quad (4)$$

where $\tilde{T}_3$ is the dimensionless form of the operator. We split $\tilde{T}_3$ into Hermitian components corresponding to the toroidal coordinates:

$$\tilde{T}_3 \equiv \tilde{T}_3^{(\theta)} + \tilde{T}_3^{(\xi)}, \quad (5)$$

which, in the limit $\alpha_\xi \rightarrow 0$ (thin torus approximation), take the form

$$\tilde{T}_3^{(\theta)} = \left\{ [3\alpha \cos^2 \theta + 2(\alpha^2 + 1) \cos \theta + \alpha] \left(\frac{i}{\alpha} \frac{\partial}{\partial \theta} + \tilde{A}_\theta \right) - \tilde{T}_\theta \right\}, \quad (6a)$$

$$\tilde{T}_3^{(\xi)} = \left\{ \sin \theta (3\alpha \cos \theta + \alpha^2 + 2) \left(i \frac{\partial}{\partial \alpha_\xi} + \tilde{A}_\xi \right) - \tilde{T}_\xi \right\}, \quad (6b)$$

$$\begin{aligned} \tilde{T}_\theta &= i \frac{\sin \theta [9\alpha^2 \cos^2 \theta + 2\alpha(2\alpha^2 + 5) \cos \theta + 3\alpha^2 + 2]}{2(1 + \alpha \cos \theta) \alpha} \\ &= -\tilde{T}_\xi. \end{aligned} \quad (6c)$$

The explicit forms of $\tilde{T}_3$ in toroidal coordinates, at arbitrary α_ξ , are given in Appendix A.2.

C. Aharonov-Bohm periodicity

If the torus has very thin walls (i.e., $\xi_{\max}/r \rightarrow 0$), the 2D dynamics governed by $\hat{\mathcal{H}}^{(2D)}$ is periodic in the intensity of the vector field. This is demonstrated by the unitary transformation:

$$\mathcal{U}(\theta, \phi, 0) \approx \exp \left[-i \int_0^\theta \alpha \tilde{A}_\theta(\theta', \phi, 0) d\theta' \right]. \quad (7)$$

Applying this transformation eliminates the vector potential from the 2D Hamiltonian:

$$\mathcal{U} \tilde{H}^{(2D)} \mathcal{U}^{-1} = \tilde{\mathcal{H}}_{\text{free}}^{(2D)} \quad (8)$$

(see Appendix A.3 for derivation details). Similarly, for the TD operator and momentum, we find

$$\mathcal{U} \tilde{T}_3^{(\theta)} \mathcal{U}^{-1} = \tilde{T}_3^{(\theta)}|_{\mathbf{A}=0} \quad \text{and} \quad \mathcal{U} \tilde{p}_\theta \mathcal{U}^{-1} = \tilde{p}_\theta^{\text{free}}. \quad (9)$$

The transformation shifts the effect of the field into the boundary conditions. The transformed wavefunctions $\psi^{(\mathcal{U})}(\theta, \phi, 0) \equiv \mathcal{U} \psi$ satisfy

$$\psi^{(\mathcal{U})}(2\pi, \phi, 0) = \exp(-i\theta_A) \psi(0, \phi, 0),$$

$$\text{where } \theta_A \equiv \int_0^{2\pi} \alpha \tilde{A}_\theta(\theta', \phi, 0) d\theta' \equiv \frac{q}{\hbar} \Phi_B. \quad (10)$$

Here, Φ_B is the magnetic flux. When $\theta_A = 2\pi n$ or $2\pi(n + 1/2)$ (where n is an integer), the system satisfies periodic or antiperiodic boundary conditions, respectively.

D. The electromagnetic field

For a straight filiform current I of length L along the z axis (Fig. 1), the dimensionless vector potential $\tilde{\mathbf{A}} \equiv (qR/\hbar)\mathbf{A}$ is

$$\begin{aligned} \tilde{A}_\phi &= 0, \quad \tilde{A}_\theta = \frac{I}{2I_0} \ln \left\{ \frac{2L}{R[1 + (\alpha + \alpha_\xi) \cos \theta]} \right\} \cos \theta, \\ \tilde{A}_\xi &= \frac{I}{2I_0} \ln \left\{ \frac{2L}{R[1 + (\alpha + \alpha_\xi) \cos \theta]} \right\} \sin \theta, \end{aligned} \quad (11)$$

where $I_0 \equiv \pi \hbar / (\mu_0 q R)$. The Aharonov-Bohm phase becomes

$$\theta_A = -2\pi \frac{I}{I_0} \frac{(a - \sqrt{a^2 - 1})}{2a}. \quad (12)$$

This defines the periodicity current I_{per} (for q equal to the electron charge):

$$I_{\text{per}} \equiv I_0 2a(a + \sqrt{a^2 - 1}) \approx \frac{2a(a + \sqrt{a^2 - 1})}{R} \times 1.6455 \times 10^{-9} \text{ A m}, \quad (13a)$$

$$\text{with } \lim_{a \rightarrow 1} [2a(a + \sqrt{a^2 - 1})] = 2 \quad \text{and} \quad 2a(a + \sqrt{a^2 - 1}) \stackrel{a \gg 1}{\approx} 4a^2. \quad (13b)$$

We plot $I_{\text{per}} R$ (in units of nA m) versus a in Fig. 2.

E. The basis vectors for the Hilbert space

We introduce the orthonormal basis functions:

$$\begin{aligned} \mathcal{F}_{n,m,k}^{(\Lambda)}(\theta, \phi, \xi) &= \frac{\sin(\pi k \alpha_\xi / \alpha_{\xi_{\max}}) e^{i(n\theta + m\phi)}}{\pi R^{3/2} \sqrt{2\alpha_{\xi_{\max}} (\alpha + \alpha_\xi) [1 + (\alpha + \alpha_\xi) \cos \theta]}} \\ &\equiv \frac{\tilde{\mathcal{F}}_{n,m,k}^{(\Lambda)}(\theta, \phi, \alpha_\xi)}{R^{3/2}}, \end{aligned} \quad (14a)$$

where $n, m \in \mathbb{Z}$ and $k \in \mathbb{N}^*$. These functions are eigenfunctions of $\hat{L}_3$ (the z projection of the angular momentum

operator) and of $\hat{p}_\theta^{\text{free}}$ in the limit $\xi_{\max} \rightarrow 0$:

$$\begin{aligned} \hat{L}_3 \mathcal{F}_{n,m,k}^{(\Lambda)} &= m \hbar \mathcal{F}_{n,m,k}^{(\Lambda)}, \\ \hat{p}_\theta^{\text{free}} \mathcal{F}_{n,m,k}^{(\Lambda)}|_{\xi_{\max} \rightarrow 0} &= \frac{n \hbar}{r} \mathcal{F}_{n,m,k}^{(\Lambda)}. \end{aligned} \quad (14b)$$

The explicit normalization condition is given in Eq. (A.7).

III. RESULTS

We calculate the matrix elements of the Hamiltonian and toroidal dipole operator $\tilde{T}_3$ in the basis [Eq. (14)]. Using these, we numerically solve the eigenvalue problem and calculate the expectation values of $\tilde{T}_3$.

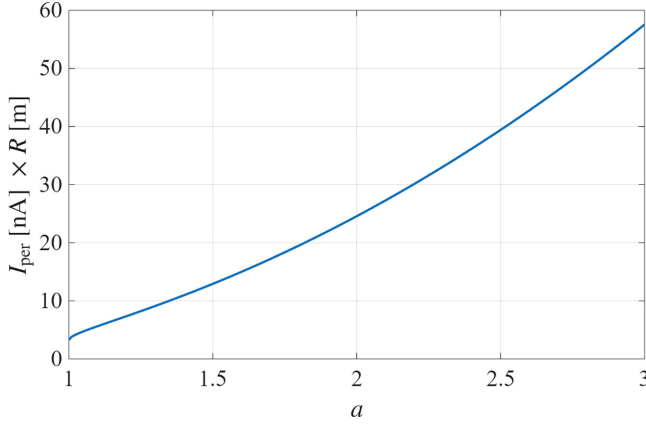


FIG. 2. The dependence of the product $I_{\text{per}}R$ (in nA m) on the parameter a . The solid curve represents the analytical behavior derived in Eq. (13a), where the geometric factor $2a(a + \sqrt{a^2 - 1})$ is scaled by the constant 1.6455×10^{-9} A m.

A. The matrix elements of the Hamiltonian

The matrix elements of the field-free 2D Hamiltonian $\tilde{\mathcal{H}}_{\text{free}}^{(2D)}$ in the limit $\alpha_{\xi_{\text{max}}} \rightarrow 0$ are

$$\begin{aligned} & \langle \tilde{\mathcal{F}}_{n_2, m, k}^{(\Lambda)} | \tilde{\mathcal{H}}_{\text{free}}^{(2D)} | \tilde{\mathcal{F}}_{n_2, m, k}^{(\Lambda)} \rangle \\ &= a^2 \left[\left(n_2^2 - \frac{1}{4} \right) + \frac{a}{(a^2 - 1)^{\frac{3}{2}}} \left(m^2 - \frac{1}{4} \right) \right], \end{aligned} \quad (15a)$$

$$\begin{aligned} & \langle \tilde{\mathcal{F}}_{n_2 - n, m, k}^{(\Lambda)} | \tilde{\mathcal{H}}_{\text{free}}^{(2D)} | \tilde{\mathcal{F}}_{n_2, m, k}^{(\Lambda)} \rangle \\ &= \frac{a^2 (|n| \sqrt{a^2 - 1} + a) (\sqrt{a^2 - 1} - a)^{|n|}}{(a^2 - 1)^{\frac{3}{2}}} \left(m^2 - \frac{1}{4} \right) \quad (n \neq 0). \end{aligned} \quad (15b)$$

The matrix elements of the transverse component is

$$\begin{aligned} & \langle \tilde{\mathcal{F}}_{n_2 - n, m, k}^{(\Lambda)} | \tilde{\mathcal{H}}_{\text{free}}^{(\xi)} | \tilde{\mathcal{F}}_{n_2, m, k'}^{(\Lambda)} \rangle \\ &= \delta_{mm'} \delta_{kk'} \delta_{n,0} \frac{\pi^2 k^2}{\alpha_{\xi_{\text{max}}}^2}, \quad \text{where } k \text{ is an integer.} \end{aligned} \quad (16)$$

In the thin-shell limit ($\alpha_{\xi_{\text{max}}} \rightarrow 0$), this energy scale dominates, freezing the system into the transverse ground state ($k = 1$). Calculating the matrix elements of the interaction terms $\tilde{\mathcal{H}}_A$, we find that all terms linear in $\alpha_{\xi_{\text{max}}}^{-1}$ vanish, and, moreover,

$$\lim_{\alpha_{\xi_{\text{max}}} \rightarrow 0} \langle \tilde{\mathcal{F}}_{n_2 - n, m, 1}^{(\Lambda)} | \tilde{\mathcal{H}}_{A,1}^{(\xi)} | \tilde{\mathcal{F}}_{n_2, m', 1}^{(\Lambda)} \rangle = 0 \quad (17)$$

(see Appendix B for detailed integrations and the expressions of all the other matrix elements). Consequently, the system is described by the effective Hamiltonian:

$$\tilde{\mathcal{H}}_{\text{eff}} \equiv \tilde{\mathcal{H}}^{(2D)} + \tilde{\mathcal{H}}_{A,2}^{(\xi)} \equiv \tilde{\mathcal{H}}^{(2D)} + \tilde{A}_{\xi}^2. \quad (18)$$

Applying the unitary transformation $\mathcal{U}$ [Eq. (7)], the eigenvalue problem reduces to solving a field-free 2D Hamiltonian subject to the flux-dependent boundary conditions [Eq. (10)], plus the scalar potential term $\tilde{A}_{\xi}^2$:

$$\tilde{\mathcal{H}}_{\text{eff}}^{(\mathcal{U})} \equiv \mathcal{U} \tilde{\mathcal{H}}_{\text{eff}} \mathcal{U}^{-1} = \tilde{\mathcal{H}}_{\text{free}}^{(2D)} + \tilde{\mathcal{H}}_{A,2}^{(\xi)}. \quad (19)$$

B. The matrix elements of the toroidal dipole

The matrix elements of the components of $\tilde{T}_3$ are calculated in Appendix B. We note that under the unitary transformation $\mathcal{U}$, the toroidal dipole operator transforms as [Eqs. (9) and (A5e)]

$$\begin{aligned} \tilde{T}_3^{(\mathcal{U})} \equiv \mathcal{U} \tilde{T}_3 \mathcal{U}^{-1} &= \tilde{T}_3^{(\theta)}|_{A=0} + \tilde{T}_{3,A}^{(\xi)} = \tilde{T}_3^{(\theta)}|_{A=0} \\ &+ \frac{2a^2 + 3a \cos \theta + 1}{a^2} \sin \theta \tilde{A}_{\xi}. \end{aligned} \quad (20)$$

This form separates the geometric contribution (first term) from the field-induced contribution (second term).

C. Numerical results

Hereafter, we explicitly emphasize the current dependence of operators by using expressions such as $\tilde{\mathcal{H}}^{(2D)}(I)$, $\tilde{\mathcal{H}}(I)$, $\tilde{T}_3^{(\theta)}(I)$, and $\tilde{T}_3(I)$. For a fixed wave vector index $k = 1$ and each azimuthal quantum number m , we numerically diagonalize the Hamiltonians $\tilde{\mathcal{H}}(I)$ and $\tilde{\mathcal{H}}^{(2D)}(I)$ within an 801-dimensional space spanned by the basis functions $\{\mathcal{F}_{n_2, m, 1}^{(\Lambda)}\}$, where n_2 ranges from -400 to 400 . The energy levels are indexed by $l = 0, 1, 2, \dots$, where $l = 0$ corresponds to the ground state, and increasing values of l represent successively higher energy levels. This basis dimensionality is sufficient to ensure numerical convergence for the examples presented below.

First, we illustrate the periodicity of the 2D dynamics, as proven in Sec. II C. Let $\tilde{E}_{l, m, 1}^{(2D)}$ and $|\tilde{\psi}_{l, m, 1}^{(2D)}(I)\rangle$ be the eigenvalues and eigenfunctions of the 2D Hamiltonian $\tilde{\mathcal{H}}^{(2D)}(I)$ for different values of a and m (with the ground state corresponding to $l = 0$):

$$\tilde{\mathcal{H}}^{(2D)}(I) |\tilde{\psi}_{l, m, 1}^{(2D)}(I)\rangle = \tilde{E}_{l, m, 1}^{(2D)} |\tilde{\psi}_{l, m, 1}^{(2D)}(I)\rangle, \quad (21a)$$

where $\tilde{E}_{l, m, 1}^{(2D)} \leq \tilde{E}_{l', m, 1}^{(2D)}$ for any $0 \leq l < l'$. Figure 3 displays $\tilde{E}_{l, m, 1}^{(2D)}/a^2$, whereas Fig. 4 shows the expectation values of $\tilde{T}_3^{(\theta)}$, normalized to $\Delta \tilde{T}_3 = 2.5$ (29), on the eigenstates $|\tilde{\psi}_{l, m, 1}^{(2D)}(I)\rangle$:

$$\frac{\langle \tilde{T}_3^{(\theta)} \rangle_{l, m, 1}^{(2D)}(I)}{\Delta \tilde{T}_3} \equiv \frac{\langle \tilde{\psi}_{l, m, 1}^{(2D)}(I) | \tilde{T}_3(I) | \tilde{\psi}_{l, m, 1}^{(2D)}(I) \rangle}{\Delta \tilde{T}_3}. \quad (21b)$$

Next, we consider the full Hamiltonian. We define $\Delta \tilde{E}_{l, m, 1}(I) \equiv \tilde{E}_{l, m, 1}(I) - \tilde{E}_{0, m, 1}(I)$, where $|\tilde{\psi}_{l, m, 1}(I)\rangle$ and $\tilde{E}_{l, m, 1}(I)$ are the eigenvectors and eigenvalues of $\tilde{\mathcal{H}}(I)$, respectively:

$$\tilde{\mathcal{H}}(I) |\tilde{\psi}_{l, m, 1}(I)\rangle = \tilde{E}_{l, m, 1}(I) |\tilde{\psi}_{l, m, 1}(I)\rangle. \quad (22)$$

By definition, $\Delta \tilde{E}_{0, m, 1}(I) \equiv 0$. The energy eigenvalues are ordered such that $\tilde{E}_{l, m, 1}(I) \leq \tilde{E}_{l', m, 1}(I)$ for $l < l'$ at any $I \geq 0$. Figure 5 plots $\Delta \tilde{E}_{l, 0, 1}(I)/a^2$ as a function of the scaled current I/I_{per} for $l = 1, \dots, 20$ (left panels) and $l = 1, \dots, 100$ (right panels), with different panels corresponding to $a = 1.2, 2$, and 3 .

Figure 6 illustrates a sudden quench scenario. The system is initially prepared in the l th energy level ($m = 0, k = 1$) at $I = 0$. The current is then quasistatically increased to a final value I , during which the system remains in the l th

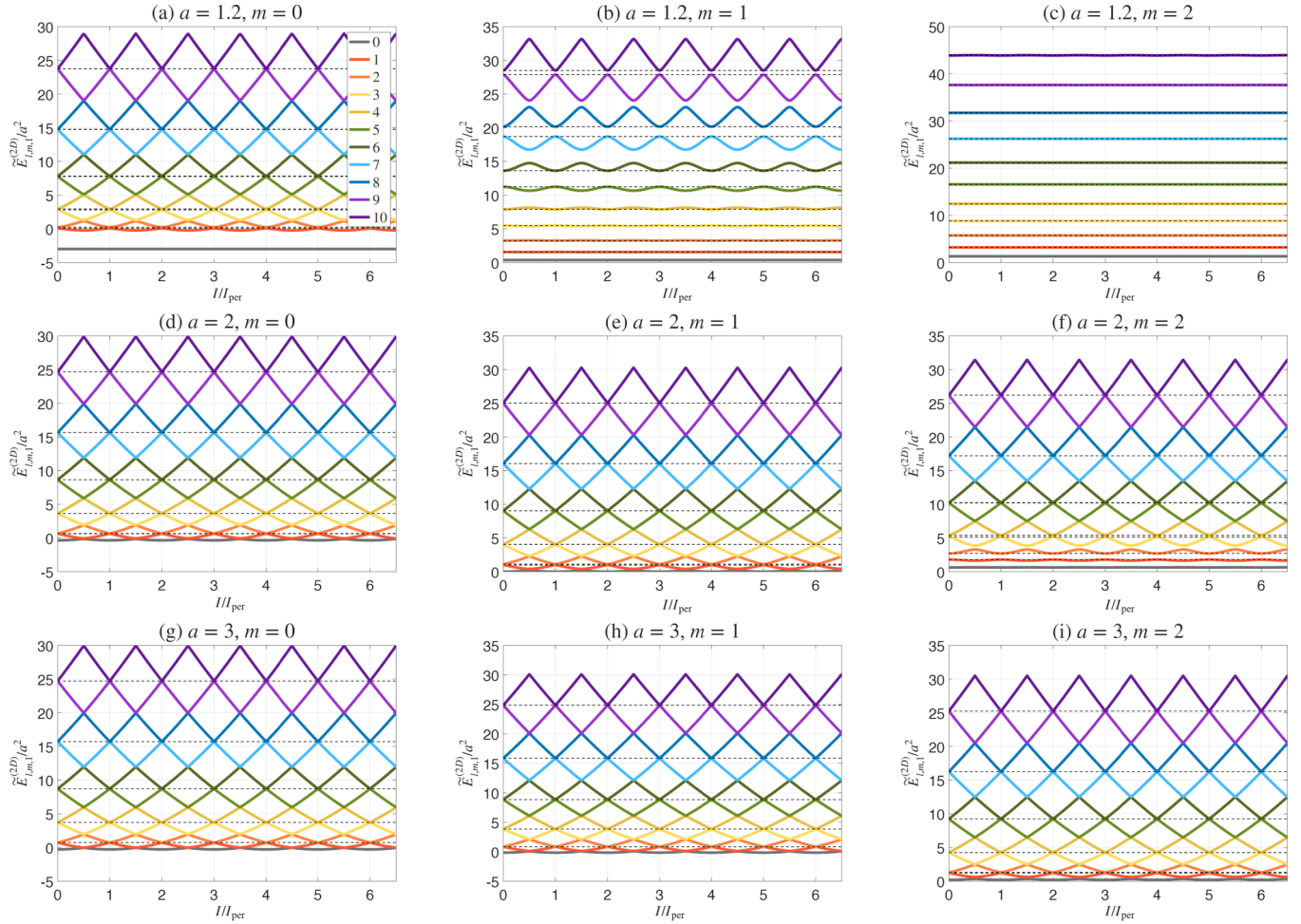


FIG. 3. Evolution of the first eleven 2D energy eigenvalues, $\tilde{E}_{l,m}^{(2D)}/a^2$ ($l = 0, \dots, 10$), as a function of the normalized current I/I_{per} . The panels are organized by the aspect ratio a (rows) and the azimuthal quantum number m (columns): top row $a = 1.2$, middle row $a = 2$, bottom row $a = 3$; left column $m = 0$, center column $m = 1$, right column $m = 2$. The color legend for the levels l , shown in the top-left panel, applies to all plots.

energy eigenstate. Subsequently, the current is instantaneously switched off (quenched) to $I = 0$. The wavefunction immediately after the quench is still $|\tilde{\psi}_{l,m,1}(I)\rangle$, but the Hamiltonian abruptly changes to $\tilde{\mathcal{H}}_{\text{free}} \equiv \tilde{\mathcal{H}}(I = 0)$ [see Eq. (3e) and Appendix A 1]. Therefore, $|\tilde{\psi}_{l,m,1}(I)\rangle$ is no longer an eigenstate, and the energy expectation value becomes $\langle \tilde{\mathcal{H}}_{\text{free}} \rangle_{l,m,1}(I) \equiv \langle \tilde{\psi}_{l,m,1}(I) | \tilde{\mathcal{H}}_{\text{free}} | \tilde{\psi}_{l,m,1}(I) \rangle$.

Figures 7 and 8 show the expectation values of $\tilde{T}_3(I)$ and $\tilde{T}_3(0)$ [where $\tilde{T}_3(0)$ is defined by Eq. (6) with $\mathbf{A} = 0$], respectively, evaluated for the energy eigenvectors $|\tilde{\psi}_{l,0,1}(I)\rangle$, scaled by $\Delta\tilde{T}_3 = 2.5$ (29), and plotted as functions of I/I_{per} . Figure 7 depicts $\langle \tilde{T}_3 \rangle_{l,0,1}(I)/\Delta\tilde{T}_3 \equiv \langle \tilde{\psi}_{l,0,1}(I) | \tilde{T}_3(I) | \tilde{\psi}_{l,0,1}(I) \rangle / \Delta\tilde{T}_3$, representing the expectation value during the quasistatic current increase. Figure 8 depicts $\langle \tilde{T}_3 \rangle_{l,0,1}^{(0)}/\Delta\tilde{T}_3 \equiv \langle \tilde{\psi}_{l,0,1}(I) | \tilde{T}_3(0) | \tilde{\psi}_{l,0,1}(I) \rangle / \Delta\tilde{T}_3$, the expectation value after the abrupt current quench. Thus, the plots in Figs. 5 and 6 have a one-to-one correspondence with those in Figs. 7 and 8, respectively. Notably, the expectation value of $\tilde{T}_3$ after the quench, $\langle \tilde{T}_3 \rangle_{l,0,1}^{(0)}(I \neq 0)$, is generally different from its initial value, $\langle \tilde{T}_3 \rangle_{l,0,1}(I = 0)$.

To illustrate the effect of the finite-dimensional basis set on the computed eigenvectors, Table I presents animations provided in the Supplemental Material [18]. Each animation shows the evolution with I of the probability amplitudes $|\langle \tilde{\psi}_{l,m,1}(I) | \tilde{\mathcal{F}}_{n_2,m,1}^{(\Lambda)} \rangle|^2$, where n_2 spans the interval $[-400, 400]$. Here, $\tilde{\psi}_{l,m,1}(I)$ denotes the eigenvector of $\tilde{\mathcal{H}}(I)$ for the l th energy level, with fixed m and $k = 1$. These animations are generated for specific a and l values, with I ranging from 0 to $10I_{\text{per}}$. The animations demonstrate the adequacy of this basis for smaller a and I values, as used in Figs. 5–8. This adequacy is evident from the vanishingly small components $|\langle \tilde{\psi}_{l,m,1}(I) | \tilde{\mathcal{F}}_{\pm 400,m,1}^{(\Lambda)} \rangle|^2$ at the boundaries ($n_2 = \pm 400$). However, for larger a or I , the basis becomes insufficient, potentially leading to numerical artifacts, as observed in the simulations from the lower part of Table I.

Finally, the initial frames of the animations, and the left panels of Figs. 7 and 8, show that $\langle \tilde{T}_3 \rangle_{l,m,1}(I = 0) = 0$. This result, rigorously proven in Appendix G, corrects numerical inaccuracies in Ref. [10], where the diagonalization yielded nonzero values, $\langle \tilde{T}_3 \rangle_{l,m,1}(I = 0) \neq 0$, for large l . These

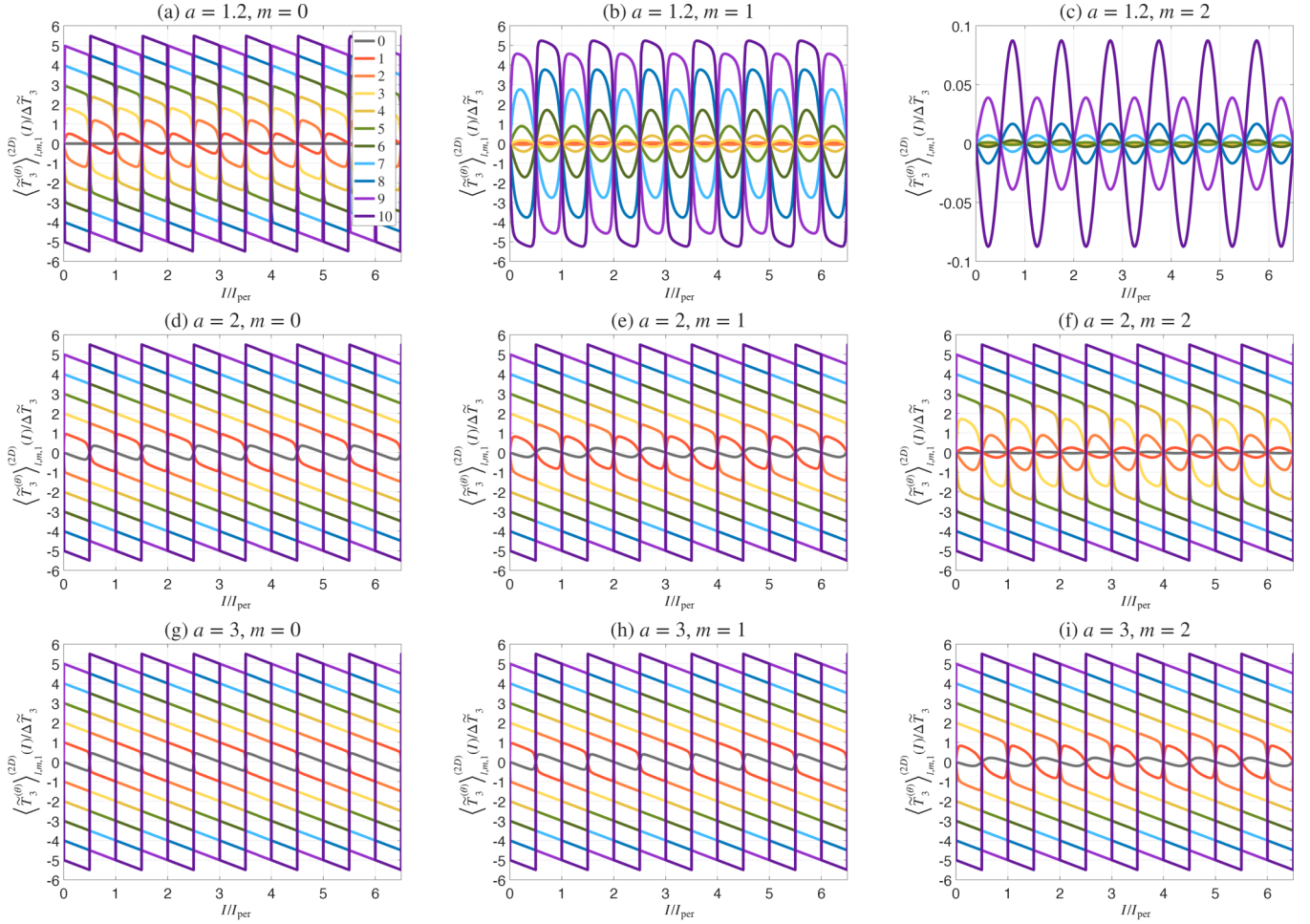


FIG. 4. Expectation values of the dimensionless toroidal dipole operator component $\tilde{T}_3^{(\theta)}$ for the first 11 eigenstates, scaled by the quantum $\Delta\tilde{T}_3 = 2.5$. The data are plotted against the normalized current I/I_{per} . The panels are arranged by aspect ratio a (rows: 1.2, 2, 3) and azimuthal quantum number m (columns: 0, 1, 2), matching the layout of Fig. 3. The color legend for the energy levels $l = 0, \dots, 10$, shown in the top-left panel, applies to all plots.

erroneous results are attributed to the quasidouble degeneracy of the corresponding energy levels, as we shall see in the next section.

D. Approximate eigensolutions and quasidegeneracy

In the absence of external current ($I = 0$), the Hamiltonian reduces to the free Hamiltonian analyzed in Refs. [10,19]. As we will show in Sec. III F, the problem is best solved on the basis of symmetric and antisymmetric wavefunctions $\{\mathcal{F}_{n_2,m,k}^{(\pm)}\}$ (31). For sufficiently large values of a or n_2 , the diagonal matrix elements dominate, and $\mathcal{F}_{n_2,m,k}^{(\pm)}$ serve as good approximations for the eigenfunctions. The ground state corresponds to $n_2 = 0$ with eigenfunction $\mathcal{F}_{0,m,k}^{(+)} \equiv \mathcal{F}_{0,m,k}^{(\Lambda)}$, while the excited states ($n_2 > 0$) appear as quasidegenerate pairs $\mathcal{F}_{n_2,m,k}^{(-)}$ and $\mathcal{F}_{n_2,m,k}^{(+)}$, corresponding to levels $2n_2 - 1$ and $2n_2$, respectively.

For an arbitrary current I , we employ the unitary transformation Eqs. (8) and (9) to map the field-dependent Hamiltonian back to the free form. To satisfy the modified boundary conditions (10), we introduce the transformed

basis:

$$\begin{aligned} \tilde{\mathcal{F}}_{n_2,m,k}^{(\Lambda,I)}(\theta, \phi, \alpha_\xi) &= \frac{\sin(\pi k \alpha_\xi / \alpha_{\xi_{\text{max}}}) \exp \left\{ i \left[\left(n_2 - \frac{\theta_A(I)}{2\pi} \right) \theta + m \phi \right] \right\}}{\pi \sqrt{2 \alpha_{\xi_{\text{max}}} (\alpha + \alpha_\xi) [1 + (\alpha + \alpha_\xi) \cos \theta]}} \\ &\equiv \tilde{\mathcal{F}}_{n_2^{(I)},m,k}^{(\Lambda)}(\theta, \phi, \alpha_\xi), \end{aligned} \quad (23)$$

where the transformed quantum number is defined as

$$n_2^{(I)} \equiv n_2 - \theta_A(I)/(2\pi) \equiv n_2 + I/I_{\text{per}}. \quad (24)$$

These functions form a complete orthonormal set. On this basis, the matrix elements of $\tilde{H}_{\text{free}}^{(2D)}$ are analogous to those in Eq. (15a), with n_2 replaced by $n_2^{(I)}$.

For sufficiently large $n_2^{(I)}$ or a , the diagonal terms dominate, yielding the approximate eigenvalues:

$$\tilde{E}_{n_2^{(I)},m,1}^{(2D)} \approx a^2 \left[\left(n_2^{(I)} \right)^2 - \frac{1}{4} + \frac{a}{(a^2 - 1)^{3/2}} \left(m^2 - \frac{1}{4} \right) \right]. \quad (25)$$

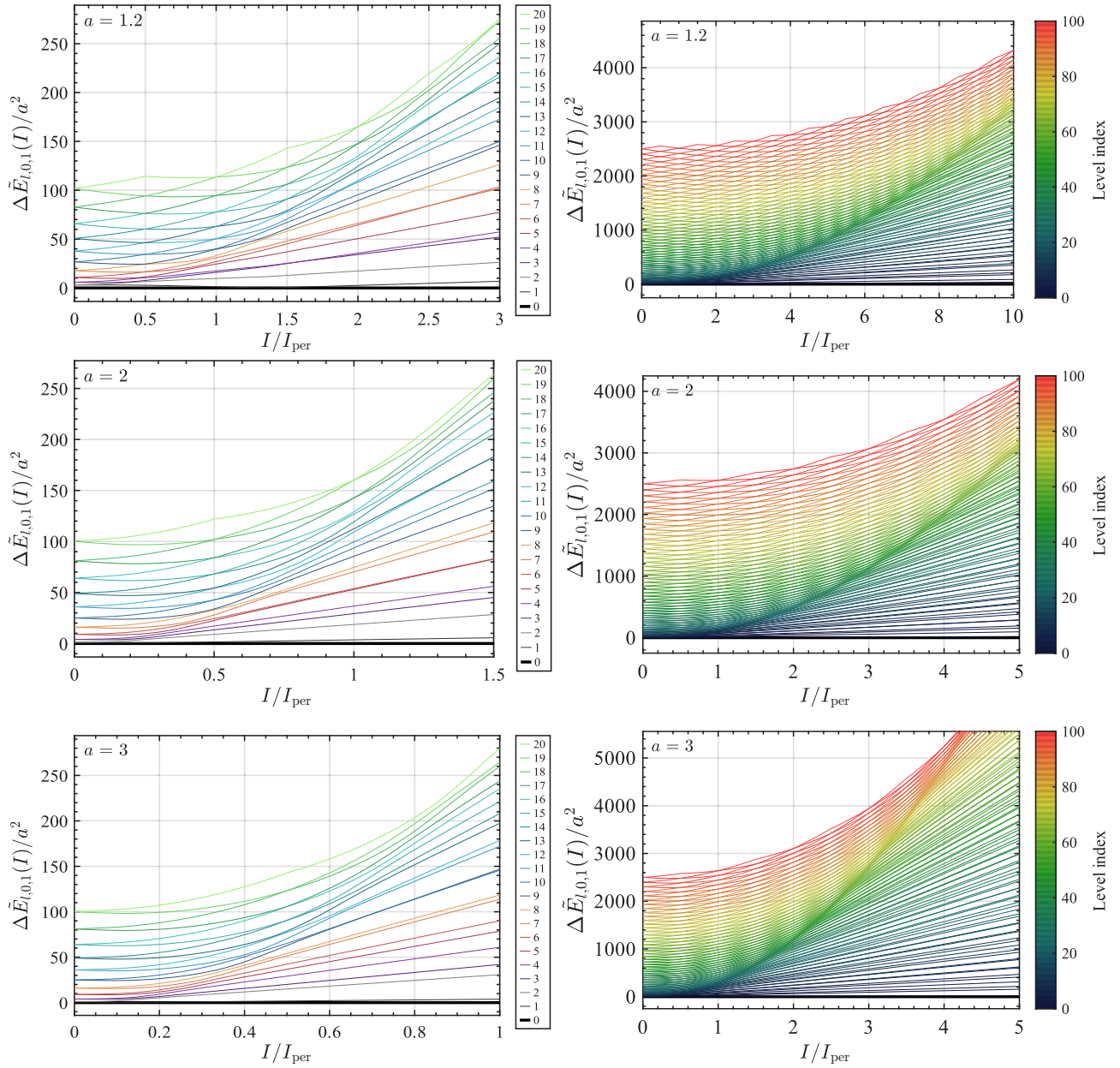


FIG. 5. Scaled excitation energies $\Delta\tilde{E}_{l,0,1}(I)/a^2$ as a function of the normalized current I/I_{per} for the azimuthal quantum number $m = 0$. The rows correspond to different aspect ratios: $a = 1.2$ (top), $a = 2$ (middle), and $a = 3$ (bottom). Left panels: Detailed view of the first 20 excited states ($l = 1, \dots, 20$). Individual levels are identified by the legend within each panel. Right panels: Extended spectrum showing the first 100 excited states ($l = 1, \dots, 100$) to illustrate the global density of states and the breakdown of quasidegeneracy at higher currents. The level index l is indicated by the color bar on the right side of each panel. Note that the detailed structure visible in the left panels is compressed into the bottom region of the right panels.

This parabolic dependence on $n_2^{(I)}$ explains the energy spectrum structure observed in Fig. 3. Unlike the $I = 0$ case, the levels $\tilde{E}_{n_2^{(I)}, m, 1}^{(2D)}$ are generally not degenerate. Degeneracy occurs only when

$$n_2 + I/I_{\text{per}} = \pm[n_2' + I/I_{\text{per}}]. \quad (26)$$

The nontrivial solution ($n_2 \neq n_2'$) requires

$$\frac{\theta_A(I)}{2\pi} \equiv -\frac{I}{I_{\text{per}}} = \frac{n_2 + n_2'}{2}, \quad (27)$$

which corresponds precisely to integer and half-integer values of I/I_{per} .

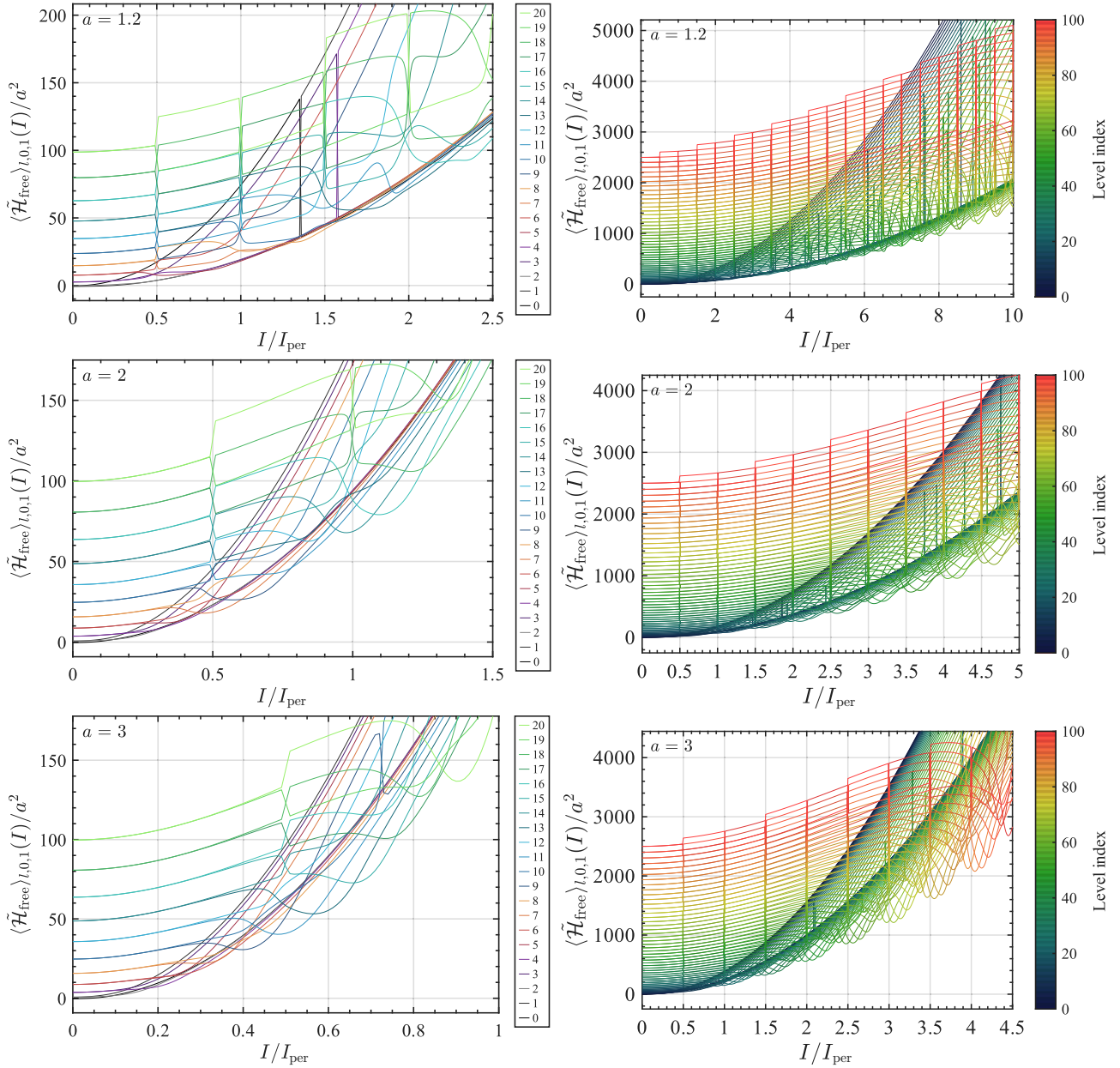


FIG. 6. Scaled expectation values of the free Hamiltonian, $\langle \tilde{\mathcal{H}}_{\text{free}} \rangle_{l,0,1}(I)/a^2$ (representing the system energy immediately after a sudden current quench to zero), plotted against the normalized initial current I/I_{per} for $m = 0$. The rows correspond to aspect ratios $a = 1.2$ (top), $a = 2$ (middle), and $a = 3$ (bottom). Left panels: Detailed evolution of the first 20 levels ($l = 1, \dots, 20$). The solid black curve tracks the state that was initially the ground state. Individual levels are identified by the legend within each panel. Right panels: Extended view including the first 100 levels ($l = 1, \dots, 100$), illustrating the complex interference patterns and level crossings in the high-energy spectrum. The level index l is indicated by the color bar on the right side of each panel.

Finally, to link the continuous parameter $n_2^{(l)}$ to the discrete energy level index l used in our plots, we derive the mapping:

$$l \equiv \begin{cases} 2\lfloor n_2^{(l)} \rfloor, & \text{if } \{n_2^{(l)} > 0, n_2^{(l)} \geq \lfloor n_2^{(l)} \rfloor\} \text{ or } \{n_2^{(l)} < 0, n_2^{(l)} < \lfloor n_2^{(l)} \rfloor\}, \\ 2\lfloor n_2^{(l)} \rfloor - 1, & \text{if } \{n_2^{(l)} < 0, n_2^{(l)} \geq \lfloor n_2^{(l)} \rfloor\} \text{ or } \{n_2^{(l)} > 0, n_2^{(l)} < \lfloor n_2^{(l)} \rfloor\}, \end{cases} \quad (28)$$

where $\lfloor x \rfloor$ denotes the nearest integer to x (with the convention that $\lfloor 0.5 \rfloor \equiv 1$ and $\lfloor -0.5 \rfloor \equiv 0$).

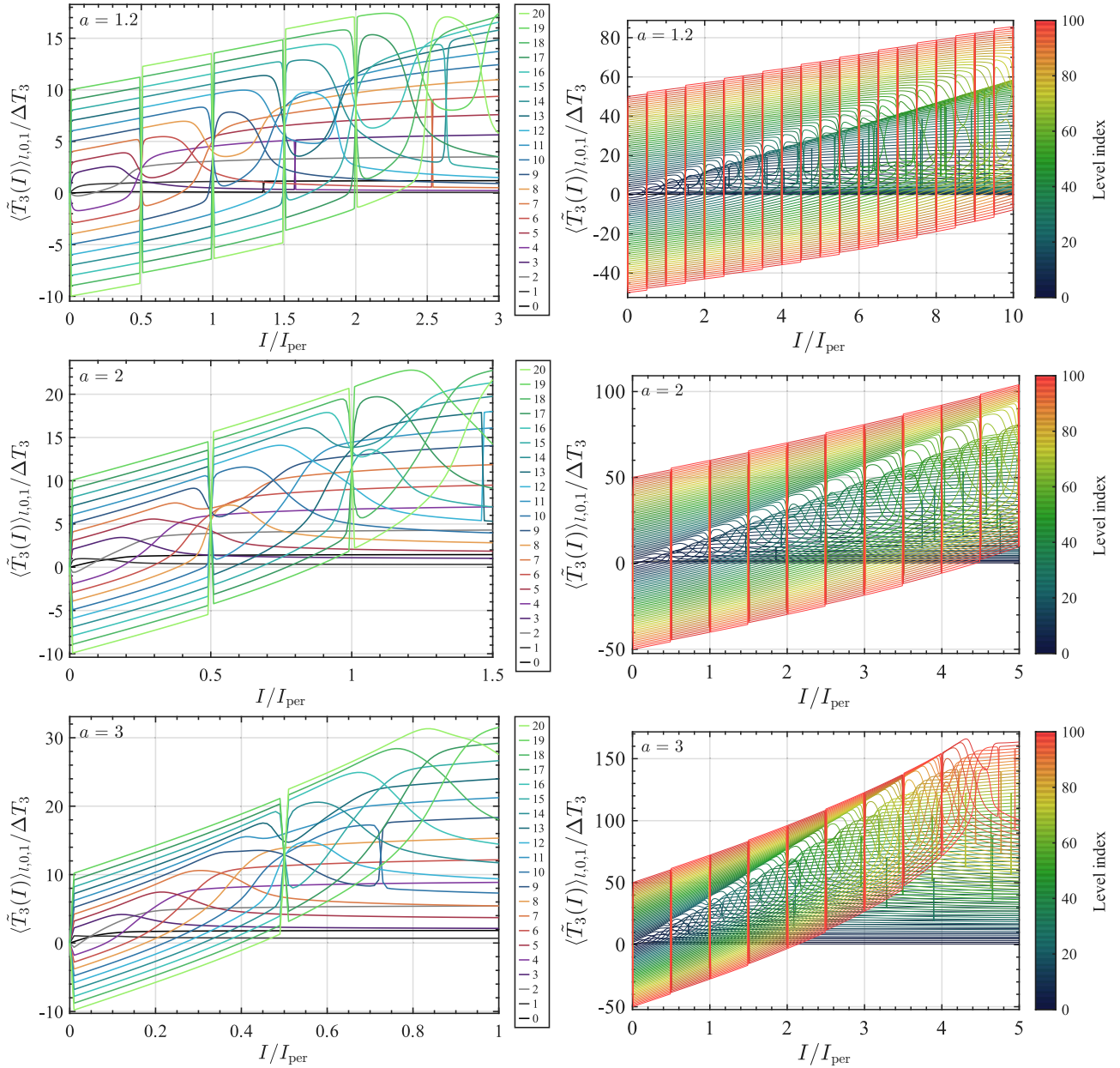


FIG. 7. Scaled expectation values of the toroidal dipole, $\langle \tilde{T}_3(I) \rangle_{l,0,1} / \Delta \tilde{T}_3$, as a function of the scaled current I/I_{per} for $m = 0$. The rows correspond to aspect ratios $a = 1.2$ (top), $a = 2$ (middle), and $a = 3$ (bottom). Left panels: Detailed evolution of the lowest 21 eigenstates ($l = 0, \dots, 20$). The black line indicates the ground state ($l = 0$). Individual levels are identified by the legend within each panel. Right panels: Extended view including states up to $l = 100$. The level index l is indicated by the color bar on the right side of each panel. The sharp discontinuities near integer and half-integer values of I/I_{per} reflect the quantization of the toroidal dipole transitions.

E. Expectation values of $\tilde{T}_3^{(\theta)}$ and quantization

Similarly, the matrix elements of $\tilde{T}_3^{(\theta)}(I)$ may be read off Eq. (B14b) [for $\tilde{T}_3^{(\theta)}(I = 0) = \tilde{T}_{3,0}^{(\xi)} + \tilde{T}_{3,0}^{(\theta)}$], replacing n_2 by $n_2^{(I)}$. Since in the Hamiltonian eigenfunctions the diagonal elements dominate, the expectation values of $\tilde{T}_3^{(\theta)}(I)$ may be approximated by

$$\langle \tilde{T}_3^{(\theta)}(I) \rangle_{l,m,1} \approx -\frac{5n_2^{(I)}(l)}{2} \equiv -\Delta \tilde{T}_3 \left(n_2(l) + \frac{I}{I_{\text{per}}} \right), \quad (29)$$

which is seen in Fig. 4 for the upper energy levels. This explicitly exposes the “quanta” of the toroidal dipole $\Delta \tilde{T}_3 \equiv 5/2$.

Combining Eq. (25) with Eq. (29), we obtain a direct relation between the energy and the toroidal dipole moment:

$$\tilde{E}_{l,m,1}^{(2D)} \approx a^2 \left[\frac{4}{25} \langle \tilde{T}_3^{(\theta)}(I) \rangle_{l,m,1}^2 - \frac{1}{4} + \frac{a}{(a^2 - 1)^{3/2}} \left(m^2 - \frac{1}{4} \right) \right]. \quad (30)$$

The abrupt changes in $\langle \tilde{T}_3^{(\theta)}(I) \rangle$ observed in Fig. 4 around $I/I_{\text{per}} = \eta/2$ arise because the mapping between the energy level index l (ordered by energy) and the quantum number n_2 switches at the degeneracy points. Specifically, as I crosses a half-integer value, the state corresponding to index l

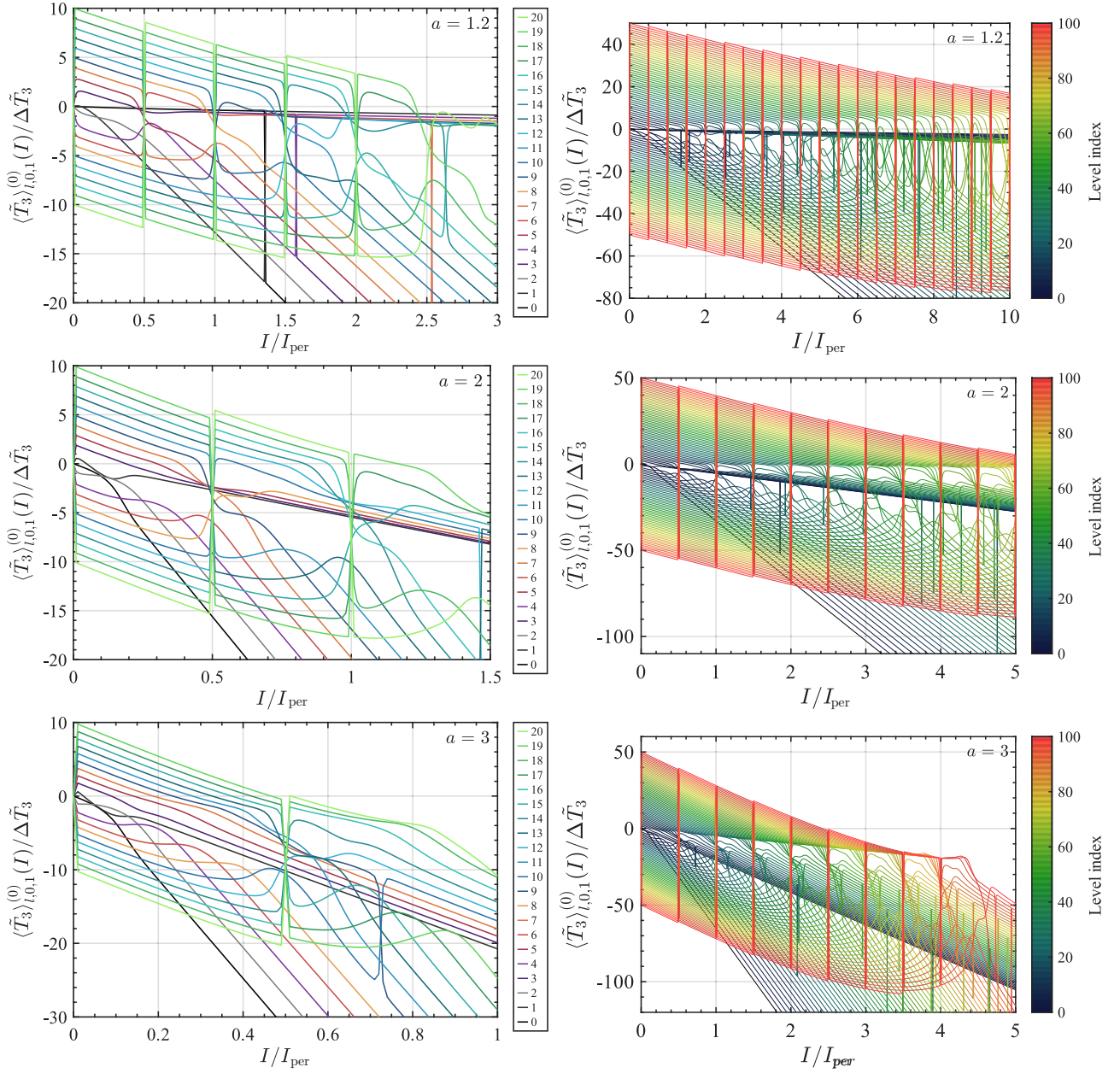


FIG. 8. Scaled expectation values of the zero-field toroidal dipole moment, $\langle \tilde{T}_3 \rangle_{l,0,1}^{(0)}(I)/\Delta \tilde{T}_3$, evaluated for the eigenstates $|\tilde{\psi}_{l,0,1}(I)\rangle$ and plotted against the scaled current I/I_{per} for $m = 0$. This quantity represents the dipole moment measured immediately after a sudden quench of the current to zero. The rows correspond to aspect ratios $a = 1.2$ (top), $a = 2$ (middle), and $a = 3$ (bottom). Left panels: Detailed evolution for the lowest 21 eigenstates ($l = 0, \dots, 20$). The solid black line indicates the ground state ($l = 0$). Individual levels are identified by the legend within each panel. Right panels: Extended view including states up to $l = 100$. The level index l is indicated by the color bar on the right side of each panel. Unlike the adiabatic dipole moment (Fig. 7), these values reflect the projection of the current-dressed states onto the zero-field operator.

switches from a positive $n_2^{(l)}$ to a negative $n_2^{(l)}$ (or vice versa), causing the expectation value to jump from $\approx 2.5(l/2)$ to $\approx -2.5(l/2)$. This switching mechanism is rigorously derived in Appendix C.

F. Symmetry and energy splitting at degeneracy points

At the special points where $I/I_{\text{per}} = \eta/2$ (with η an integer), the set of transformed quantum numbers $\{n_2^{(l)}\}$ becomes

symmetric with respect to zero. This symmetry suggests a description in terms of symmetric (+) and antisymmetric (−) basis states, defined as

$$\begin{aligned} \tilde{\mathcal{F}}_{n_2^{(l)},m,k}^{(\pm)} &\equiv \frac{1}{\sqrt{2}} [\tilde{\mathcal{F}}_{n_2^{(l)},m,k}^{(\Lambda)} \pm \tilde{\mathcal{F}}_{-n_2^{(l)},m,k}^{(\Lambda)}], \quad \text{for } n_2^{(l)} > 0, \\ \tilde{\mathcal{F}}_{0,m,k}^{(+)} &\equiv \tilde{\mathcal{F}}_{0,m,k}^{(\Lambda)}, \quad \text{and} \quad \tilde{\mathcal{F}}_{0,m,k}^{(-)} \equiv 0. \end{aligned} \quad (31)$$

TABLE I. Animations (available in the Supplemental Material [18]) depicting the squared magnitudes of the inner products, $|\langle \tilde{\psi}_{l,m,1}(I) | \tilde{\mathcal{F}}_{n_2,m,1}^{(\Lambda)} \rangle|^2$. The horizontal axis represents the basis function index n_2 (ranging from -400 to 400), and the animations show the evolution as the adiabatic parameter I increases from 0 to $10I_{\text{per}}$.

File name	a	l
Eigenvector_a1.2_m0_level1i_per0-10_max_x100.gif	1.2	1
Eigenvector_a1.2_m0_level21i_per0-10_max_x200.gif	1.2	21
Eigenvector_a1.2_m0_level101i_per0-10_max_x200.gif	1.2	101
Eigenvector_a2_m0_level1i_per0-10_max_x200.gif	2	1
Eigenvector_a2_m0_level21i_per0-10_max_x200.gif	2	21
Eigenvector_a2_m0_level101i_per0-10_max_x400.gif	2	101
Eigenvector_a3_m0_level1i_per0-10_max_x400.gif	3	1
Eigenvector_a3_m0_level21i_per0-10_max_x400.gif	3	21
Eigenvector_a3_m0_level101i_per0-10_max_x400.gif	3	101
Eigenvector_a5_m0_level1i_per0-10_max_x400.gif	5	1
Eigenvector_a5_m0_level21i_per0-10_max_x400.gif	5	21
Eigenvector_a5_m0_level101i_per0-10_max_x400.gif	5	101
Eigenvector_a10_m0_level1i_per0-10_max_x400.gif	10	1
Eigenvector_a10_m0_level21i_per0-10_max_x400.gif	10	21
Eigenvector_a10_m0_level101i_per0-10_max_x400.gif	10	101
Eigenvector_a20_m0_level1i_per0-10_max_x400.gif	20	1
Eigenvector_a20_m0_level21i_per0-10_max_x400.gif	20	21
Eigenvector_a20_m0_level101i_per0-10_max_x400.gif	20	101

The Hamiltonian $\tilde{\mathcal{H}}^{(2D)}$ does not couple symmetric and anti-symmetric states:

$$\langle \tilde{\mathcal{F}}_{n_1^{(+)},m_1,k_1}^{(+)} | \tilde{\mathcal{H}}_{\text{free}}^{(2D)} | \tilde{\mathcal{F}}_{n_2^{(-)},m_2,k_2}^{(-)} \rangle = 0. \quad (32)$$

Consequently, the energy eigenfunctions at these points have definite parity [they are entirely within the $(+)$ or $(-)$ subspace]. Crucially, the toroidal dipole operator $\tilde{T}_3$ has non-vanishing matrix elements *only* between states of opposite parity (see Appendix G). Therefore, its expectation value in any eigenstate of definite parity must vanish:

$$\langle \psi^{(\pm)} | \tilde{T}_3 | \psi^{(\pm)} \rangle = 0. \quad (33)$$

This rigorous symmetry argument explains the numerical result in Fig. 4, where $\langle \tilde{T}_3 \rangle$ passes exactly through zero at integer and half-integer values of I/I_{per} .

Furthermore, the mixing of the $\pm n_2^{(I)}$ states in the basis functions $\tilde{\mathcal{F}}_{n_2^{(I)},m_1,k_1}^{(+)}$ lifts the degeneracy predicted by the simple quadratic approximation (see Appendix G). The energy splitting is approximated by

$$\begin{aligned} \Delta \tilde{E}_{n_2^{(I)},m,1}^{(2D)} \Big|_{I/I_{\text{per}}=\eta/2} &= \frac{2a^2(2n_2^{(I)}\sqrt{a^2-1}+a)(\sqrt{a^2-1}-a)^{2n_2^{(I)}}}{(a^2-1)^{\frac{3}{2}}} \left(m^2 - \frac{1}{4} \right). \end{aligned} \quad (34)$$

This splitting decreases exponentially with $n_2^{(I)}$, explaining why the levels appear degenerate for large quantum numbers but are distinct for low-lying states.

G. The full 3D problem and transition energies

Finally, we analyze the full effective Hamiltonian [Eq. (18)], which includes the quadratic scalar potential term $\tilde{A}_\xi^2$. The system remains in the quasi-2D regime provided that the matrix elements of $\tilde{\mathcal{H}}^{(2D)}$ are large compared to those of $\tilde{\mathcal{H}}_{\Lambda,2}^{(\xi)}$. Furthermore, as long as the diagonal matrix elements of the free Hamiltonian dominate (which holds for sufficiently large a or energy level l), the quasidouble degeneracy at $I/I_{\text{per}} = \eta/2$ observed in Fig. 5 and analyzed in Sec. III F is preserved.

For small currents [according to Appendix D, $(I/I_{\text{per}})^2 \ll [\mathcal{R}^{(\xi)}(a, n_2, 2, m)]^{-1}$], the contribution from the diagonal terms is dominant and the eigenfunctions are well approximated by $\tilde{\mathcal{F}}_{n_2,m,k}^{(\Lambda)}$ or $\tilde{\mathcal{F}}_{n_2,m,k}^{(\pm)}$ if $I/I_{\text{per}} = \eta/2$, as explained in Sec. III F. In such a case, all the properties of the energy spectrum discussed in Secs. III D–III F are satisfied, except for the periodicity, since

$$\tilde{E}_{n_2^{(I)},m,1} \approx \tilde{E}_{n_2^{(I)},m,1}^{(2D)} + \frac{I^2}{I_{\text{per}}^2} a^2 h_0(a; L/R), \quad (35)$$

where $h_0(a; L/R)$ is a geometric coefficient derived in Appendix D. Similarly, the expectation value of the toroidal dipole acquires a linear correction in I :

$$\begin{aligned} \langle \tilde{T}_3 \rangle_{l,m,1} &\approx -\frac{5n_2^{(I)}(l)}{2} + \frac{I}{I_{\text{per}}} \left\{ \frac{(1+2a^2)}{2a(a-\sqrt{a^2-1})} \right. \\ &\quad \times \ln \left[\frac{4aL}{R(a+\sqrt{a^2-1})} \right] \\ &\quad \left. + \frac{1}{4a(a-\sqrt{a^2-1})} - \frac{3}{2} \right\}. \end{aligned} \quad (36)$$

While the absolute value of the toroidal dipole depends on the current, the *change* in the dipole moment between energy levels remains quantized. Substituting these expressions into the energy difference between two levels l_1 and l_2 , the quadratic terms in I cancel, leading to a remarkably simple linear relation for the transition energy:

$$\begin{aligned} \Delta \tilde{E}_{l_2,l_1} &= a^2 [n_2^2(l_2) - n_2^2(l_1)] \\ &\quad - \frac{I}{I_{\text{per}}} \frac{4a^2}{5} [\langle \tilde{T}_3 \rangle_{l_2,m,1} - \langle \tilde{T}_3 \rangle_{l_1,m,1}] \\ &= a^2 \left\{ [n_2^2(l_2) - n_2^2(l_1)] + 2 \frac{I}{I_{\text{per}}} [n_2(l_2) - n_2(l_1)] \right\}. \end{aligned} \quad (37)$$

Equation (37) is our main result: The transition energy is linear in I/I_{per} , and the slope is quantized in units of $2a^2$. This slope is directly proportional to the jump in the toroidal dipole quantum number, providing a robust spectroscopic method to measure $\tilde{T}_3$.

H. Physical validity and experimental observation

The validity of separating the dynamics into 2D rotational and transverse components—and consequently the effective Hamiltonian derived in Eq. (18)—relies on the “thin-shell”

limit. Physically, this approximation holds when the confinement energy in the transverse direction (ξ), $\tilde{E}^{(\xi)}$, far exceeds the characteristic energies of the rotational motion along the torus surface, $\tilde{E}^{(2D)}$. From Eq. (16), the lowest excitation energy in the ξ direction is

$$\Delta\tilde{E}_{\min}^{(\xi)} = 3\pi^2/\alpha_{\xi_{\max}}^2. \quad (38)$$

This energy gap must be much larger than the typical energy scale for the level l . Using the approximation for the 2D energy levels from Eq. (35), the condition $\tilde{E}^{(2D)} \ll \Delta\tilde{E}_{\min}^{(\xi)}$ becomes

$$a^2 \left[\frac{l^2 - 1}{4} + \frac{a}{(a^2 - 1)^{3/2}} \left(m^2 - \frac{1}{4} \right) \right] + \frac{I^2}{I_{\text{per}}^2} a^2 h_0(a; L/R) \ll \frac{3\pi^2}{\alpha_{\xi_{\max}}^2}. \quad (39)$$

For large a , using the asymptotic form of h_0 from Eq. (D4a), this inequality simplifies to

$$\frac{l^2}{4} + \frac{I^2}{I_{\text{per}}^2} 2 \ln^2 \left(\frac{2L}{R} \right) \ll 3\pi^2 \frac{r^2}{\xi_{\max}^2}. \quad (40)$$

This relation establishes the upper limit for the applicability of the 2D approximation. It explicitly shows that for higher energy levels (l) or stronger currents (I), a thinner shell (larger ratio $r/\xi_{\max}$) is required to maintain validity. For example, to observe the periodicity up to $I = I_{\text{per}}$ for a given level l , the geometric parameters must satisfy

$$\frac{r}{\xi_{\max}} \gg \frac{1}{\sqrt{3}\pi} \sqrt{\frac{l^2}{4} + 2 \ln^2 \left(\frac{2L}{R} \right)}. \quad (41)$$

A separate validity condition concerns the approximation of the energy levels by the diagonal matrix elements of the three-dimensional (3D) correction term. This approximation holds when the off-diagonal coupling is small compared to the energy level spacing. Using the ratio $\mathcal{R}^{(\xi)}$ defined in Appendix D [Eq. (D8d)] and the asymptotic form of h_2 [Eq. (D4c)], we estimate the breakdown condition as

$$\left| \frac{h_2(a; L/R)}{n_2^2 - \frac{1}{4}} \right| \gg \frac{I^2}{I_{\text{per}}^2} \left| \frac{\ln^2 \left(\frac{2L}{R} \right) - 2 \ln^2(a)}{n_2^2 - \frac{1}{4}} \right| \ll 1. \quad (42)$$

Comparing this estimate with the numerical results in Fig. 5 (e.g., for $a = 3$, $m = 0$), we observe that for high levels ($l \approx 20$, corresponding to $n_2 \approx 10$), the quasidegeneracy indeed begins to lift as I approaches I_{per} , consistent with the ratio in Eq. (42) becoming non-negligible (~ 0.1).

Our theoretical model finds its most direct realization in nanostructures that possess a hollow or core-shell geometry, confining carriers to a toroidal surface rather than a volume. The ideal realization is represented by *single-walled carbon nanotube tori* [14,15]. In these systems, electrons are confined to the graphene lattice (the torus surface) with a tube diameter $d \approx 1\text{--}2$ nm and a ring radius $R \approx 300\text{--}500$ nm. A second realization is provided by *bent core-shell nanowires* [16,20]. If a nanowire with an insulating core and a conductive shell is bent into a loop, the carriers are confined to a toroidal shell, matching the topology of our Hamiltonian. Finally, *TI nanorings* provide a fundamental realization of

surface-only confinement [17]. Since the bulk is insulating and the conducting states are topologically protected to exist only on the surface, the physical system naturally enforces the constraint assumed in our model. While standard *self-assembled semiconductor quantum rings* (e.g., InGaAs) are typically solid tori [12], they essentially reproduce the same rotational dynamics (Aharonov-Bohm oscillations), although the transverse energy spectrum differs from the thin-shell model.

Regarding the experimental observability of the predicted effects, the magnitude is governed by the characteristic current I_0 defined in Sec. IID:

$$I_0 \equiv \frac{\pi \hbar}{\mu_0 q R} \approx \frac{1.64 \times 10^{-9} \text{ A m}}{R}. \quad (43)$$

For a mesoscopic ring with $R \approx 1 \mu\text{m}$, the characteristic current is $I_0 \approx 1.6$ mA, which is well within the range of standard laboratory current sources. For nanoscale systems ($R \approx 20$ nm), the current increases to $I_0 \approx 80$ mA. While high, this is achievable in pulsed operation modes to mitigate heating. Crucially, the spectroscopic signature—the slope of the transition energy in Eq. (37)—is linear in I . Therefore, the quantization of the toroidal dipole can be detected by measuring the slope at currents $I < I_0$, without necessarily reaching the full periodicity current I_{per} .

IV. CONCLUSIONS

In this work, we have provided a complete theoretical framework for the quantum TD in a nanostructure and proposed a method for its direct, quantitative measurement. This resolves a foundational challenge that has persisted since the toroidal multipole family was conceptualized over 60 yr ago.

Our approach is centered on linking the TD to a direct spectroscopic observable. By analyzing a quantum particle on a toroidal manifold, we demonstrated that an external current I , acting as a conjugate field, shifts the system's energy eigenvalues. The central result of this paper is the proof that this energy shift is directly proportional to the expectation value of the TD operator. We find that the transition energy ΔE between two eigenstates is linear in the applied current, following the simple relation $\Delta E \approx C_1 + C_2 I$, where the slope C_2 is directly proportional to the change in the toroidal dipole moment between the states, $\Delta \langle \hat{T}_3 \rangle$.

This finding provides a clear and unambiguous “smoking gun” for experiment. We have shown that the toroidal dipole, in a quantum-mechanical system, is quantized. The slope of the transition energy versus current is not continuous but is determined by the discrete quantum numbers of the eigenstates. Measuring this slope provides a direct, quantitative value for the TD, in contrast to all previous indirect methods, which rely on far-field scattering and simulation.

We have explicitly addressed the physical validity of our effective 2D Hamiltonian, establishing analytical criteria for the “thin-shell” limit where transverse confinement energies dominate rotational dynamics. We demonstrated that these conditions are satisfied in realistic nanoscopic systems. Furthermore, we identified specific experimental platforms that naturally enforce this surface confinement,

including single-walled carbon nanotube tori [14,15] and topological insulator nanorings [17]. Our estimates indicate that for systems with radii ranging from 20 nm to 1 μm , the characteristic currents required to observe these spectroscopic signatures lie within the accessible milliamperage range ($I \sim 1\text{--}80$ mA).

This work bridges the gap between the classical, macroscopic toroidal dipoles studied in metamaterials and the fundamental quantum nature of matter. It builds directly upon our previous work [10,11], which established the toroidal dipole operator as a self-adjoint (Hermitian) quantum observable. Having established it as an observable in theory, we now provide the practical blueprint to observe it in an experiment.

The ability to measure and control the quantum TD opens significant avenues for research, from engineering quantum metamaterials with electromagnetic properties to probing fundamental physics, such as parity-violating anapole moments in molecules. By providing the tools to measure what was

once hidden, this work completes the quantum multipole toolkit.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [18].

APPENDIX A: EXPLICIT MATHEMATICAL EXPRESSIONS OF THE THEORETICAL FRAMEWORK

1. Hamiltonian operators

The Hermitian components of the dimensionless canonical momentum $\tilde{\mathbf{p}}_{\text{free}}$ in toroidal coordinates are

$$\tilde{p}_{\text{free}}^{(\theta)} = -i \left[\frac{1}{\alpha + \alpha_\xi} \frac{\partial}{\partial \theta} - \frac{1}{2} \frac{\sin \theta}{1 + (\alpha + \alpha_\xi) \cos \theta} \right], \quad (\text{A1a})$$

$$\tilde{p}_{\text{free}}^{(\phi)} = -i \frac{1}{1 + (\alpha + \alpha_\xi) \cos \theta} \frac{\partial}{\partial \phi}, \quad (\text{A1b})$$

$$\tilde{p}_{\text{free}}^{(\xi)} = -i \left\{ \frac{\partial}{\partial \alpha_\xi} + \frac{1 + 2(\alpha + \alpha_\xi) \cos \theta}{2(\alpha + \alpha_\xi)[1 + (\alpha + \alpha_\xi) \cos \theta]} \right\}. \quad (\text{A1c})$$

The explicit components of the field-free Hamiltonian $\tilde{\mathcal{H}}_{\text{free}}$ (3e) are

$$\tilde{\mathcal{H}}_{\text{free}}^{(\xi)} = - \left(\frac{\partial^2}{\partial \alpha_\xi^2} + \frac{1 + 2(\alpha + \alpha_\xi) \cos \theta}{2(\alpha + \alpha_\xi)[1 + (\alpha + \alpha_\xi) \cos \theta]} \frac{\partial}{\partial \alpha_\xi} - \frac{1}{4(\alpha + \alpha_\xi)^2 [1 + (\alpha + \alpha_\xi) \cos \theta]^2} \right), \quad (\text{A2a})$$

$$\begin{aligned} \tilde{\mathcal{H}}_{\text{free}}^{(2D)} = & - \left(\frac{1}{(\alpha + \alpha_\xi)^2} \frac{\partial^2}{\partial \theta^2} - \frac{\sin \theta}{(\alpha + \alpha_\xi)[1 + (\alpha + \alpha_\xi) \cos \theta]} \frac{\partial}{\partial \theta} + \frac{1}{4[1 + (\alpha + \alpha_\xi) \cos \theta]^2 (\alpha + \alpha_\xi)^2} \right) \\ & - \frac{1}{[1 + (\alpha + \alpha_\xi) \cos \theta]^2} \frac{\partial^2}{\partial \phi^2}. \end{aligned} \quad (\text{A2b})$$

The linear ($\tilde{\mathcal{H}}_{\text{A},1}$) and quadratic ($\tilde{\mathcal{H}}_{\text{A},2}$) interaction terms (3d) are decomposed as

$$\tilde{\mathcal{H}}_{\text{A},1}^{(2D)} = 2i \left[\frac{\tilde{A}_\theta}{\alpha + \alpha_\xi} \frac{\partial}{\partial \theta} + \frac{\tilde{A}_\phi}{1 + (\alpha + \alpha_\xi) \cos \theta} \frac{\partial}{\partial \phi} \right] + i \frac{\partial \{ [1 + (\alpha + \alpha_\xi) \cos \theta] \tilde{A}_\theta \} / \partial \theta + (\alpha + \alpha_\xi) \partial \tilde{A}_\phi / \partial \phi}{(\alpha + \alpha_\xi)[1 + (\alpha + \alpha_\xi) \cos \theta]}, \quad (\text{A3a})$$

$$\tilde{\mathcal{H}}_{\text{A},2}^{(2D)} = \tilde{A}_\theta^2 + \tilde{A}_\phi^2, \quad (\text{A3b})$$

$$\tilde{\mathcal{H}}_{\text{A},1}^{(\xi)} = 2i \left(\tilde{A}_\xi \frac{\partial}{\partial \alpha_\xi} + \frac{1}{2(\alpha + \alpha_\xi)[1 + (\alpha + \alpha_\xi) \cos \theta]} \frac{\partial \{ (\alpha + \alpha_\xi)[1 + (\alpha + \alpha_\xi) \cos \theta] \tilde{A}_\xi \}}{\partial \alpha_\xi} \right), \quad (\text{A3c})$$

$$\tilde{\mathcal{H}}_{\text{A},2}^{(\xi)} = \tilde{A}_\xi^2. \quad (\text{A3d})$$

2. Toroidal dipole operators

The full expression of the toroidal dipole operator in toroidal coordinates is

$$\tilde{T}_3 = -i \frac{[z \rho \hat{\mathbf{p}} - (2\rho^2 + z^2) \hat{\mathbf{z}}]}{R^2} \left[\hat{\boldsymbol{\theta}} \left(\frac{1}{\alpha + \alpha_\xi} \frac{\partial}{\partial \theta} - i \tilde{A}_\theta \right) + \hat{\boldsymbol{\xi}} \left(\frac{\partial}{\partial \alpha_\xi} - i \tilde{A}_\xi \right) \right], \quad (\text{A4})$$

where $z = (r + \xi) \sin \theta$ and $\rho \equiv R + (r + \xi) \cos \theta$ are the cylindrical coordinates, whereas $\hat{z} \equiv \hat{\theta} \cos \theta + \hat{\xi} \sin \theta$ and $\hat{\rho} \equiv -\hat{\theta} \sin \theta + \hat{\xi} \cos \theta$ are the unit vectors along them. We split $\tilde{T}_3$ into its hermitic components [10]

$$\tilde{T}_3^{(\theta)} = \tilde{T}_{3,0}^{(\theta)} + \tilde{T}_{3,A}^{(\theta)} - \tilde{T}_\theta, \quad (\text{A5a})$$

$$\tilde{T}_3^{(\xi)} = \tilde{T}_{3,0}^{(\xi)} + \tilde{T}_{3,A}^{(\xi)} - \tilde{T}_\xi, \quad (\text{A5b})$$

where

$$\tilde{T}_\theta = i \frac{\sin \theta \{9(\alpha + \alpha_\xi)^2 \cos^2 \theta + 2(\alpha + \alpha_\xi)[2(\alpha + \alpha_\xi)^2 + 5] \cos \theta + 3(\alpha + \alpha_\xi)^2 + 2\}}{2(1 + (\alpha + \alpha_\xi) \cos \theta)(\alpha + \alpha_\xi)} = -\tilde{T}_\xi, \quad (\text{A5c})$$

$$\tilde{T}_{3,0}^{(\theta)} \equiv i \left\{ 3 \cos^2 \theta + \frac{2[(\alpha + \alpha_\xi)^2 + 1] \cos \theta}{\alpha + \alpha_\xi} + 1 \right\} \frac{\partial}{\partial \theta}, \quad \tilde{T}_{3,A}^{(\theta)} \equiv \left\{ 3 \cos^2 \theta + \frac{2[(\alpha + \alpha_\xi)^2 + 1] \cos \theta}{(\alpha + \alpha_\xi)} + 1 \right\} (\alpha + \alpha_\xi) \tilde{A}_\theta, \quad (\text{A5d})$$

$$\tilde{T}_{3,0}^{(\xi)} \equiv i \sin \theta [3(\alpha + \alpha_\xi) \cos \theta + (\alpha + \alpha_\xi)^2 + 2] \frac{\partial}{\partial \alpha_\xi}, \quad \tilde{T}_{3,A}^{(\xi)} \equiv \sin \theta [3(\alpha + \alpha_\xi) \cos \theta + (\alpha + \alpha_\xi)^2 + 2] \tilde{A}_\xi. \quad (\text{A5e})$$

3. Periodicity transformation details

The unitary transformation $\mathcal{U}$ applied to the 2D Hamiltonian terms yields

$$-\mathcal{U} \frac{1}{\alpha^2} \frac{\partial^2}{\partial \theta^2} \mathcal{U}^{-1} = A_\theta^2(\theta) - \frac{i}{\alpha} \frac{\partial A_\theta(\theta)}{\partial \theta} - \frac{2i A_\theta(\theta)}{\alpha} \frac{\partial}{\partial \theta} - \frac{1}{\alpha^2} \frac{\partial^2}{\partial \theta^2}, \quad (\text{A6a})$$

$$\mathcal{U} \frac{\sin \theta}{\alpha(1 + \alpha \cos \theta)} \frac{\partial}{\partial \theta} \mathcal{U}^{-1} = i \frac{\sin \theta A_\theta(\theta)}{(1 + \alpha \cos \theta)} + \frac{\sin \theta}{\alpha(1 + \alpha \cos \theta)} \frac{\partial}{\partial \theta}, \quad (\text{A6b})$$

$$\mathcal{U} \frac{2i \tilde{A}_\theta}{\alpha} \frac{\partial}{\partial \theta} \mathcal{U}^{-1} = -2\tilde{A}_\theta^2 + \frac{2i \tilde{A}_\theta}{\alpha} \frac{\partial}{\partial \theta}, \quad (\text{A6c})$$

$$\frac{i}{\alpha(1 + \alpha \cos \theta)} \frac{\partial}{\partial [\tilde{A}_\theta(1 + \alpha \cos \theta)]} \theta = \frac{i}{\alpha} \frac{\partial}{\partial \tilde{A}_\theta} \theta - \frac{i \sin \theta}{(1 + \alpha \cos \theta)} \tilde{A}_\theta. \quad (\text{A6d})$$

Summing these contributions leads to the cancellation of all $\tilde{A}_\theta$ terms, recovering $\tilde{\mathcal{H}}_{\text{free}}^{(2D)}$.

4. Normalization of basis vectors

The normalization condition for the basis functions in toroidal coordinates is explicitly

$$\langle \tilde{\mathcal{F}}_{n,m,k}^{(\Lambda)} | \tilde{\mathcal{F}}_{n',m',k'}^{(\Lambda)} \rangle \equiv \int_0^{2\pi} d\theta \int_0^{2\pi} d\phi \int_0^{\alpha_{\xi\max}} d\alpha_\xi (\alpha + \alpha_\xi) [1 + (\alpha + \alpha_\xi) \cos \theta] (\tilde{\mathcal{F}}_{n,m,k}^{(\Lambda)}(\theta, \phi, \alpha_\xi))^* \tilde{\mathcal{F}}_{n',m',k'}^{(\Lambda)}(\theta, \phi, \alpha_\xi) = \delta_{nn'} \delta_{mm'} \delta_{kk'}. \quad (\text{A7})$$

APPENDIX B: CALCULATIONS OF MATRIX ELEMENTS

1. Hamiltonian matrix elements

To calculate the matrix elements of $\tilde{\mathcal{H}}_A$, we plug Eq. (11) into Eq. (A3) and obtain

$$\tilde{\mathcal{H}}_{A,1}^{(2D)} \equiv \frac{iL}{I_0} \left(\frac{1}{\alpha + \alpha_\xi} \ln \left[\frac{1}{1 + (\alpha + \alpha_\xi) \cos \theta} \frac{2L}{R} \right] \left\{ \cos \theta \frac{\partial}{\partial \theta} - \frac{\sin \theta [1 + 2(\alpha + \alpha_\xi) \cos \theta]}{2[1 + (\alpha + \alpha_\xi) \cos \theta]} \right\} + \frac{1}{4} \frac{\sin(2\theta)}{1 + (\alpha + \alpha_\xi) \cos \theta} \right), \quad (\text{B1a})$$

$$\tilde{\mathcal{H}}_{A,2}^{(2D)} \equiv \frac{I^2}{4I_0^2} \ln^2 \left[\frac{1}{1 + (\alpha + \alpha_\xi) \cos \theta} \frac{2L}{R} \right] \cos^2 \theta, \quad (\text{B1b})$$

$$\tilde{\mathcal{H}}_{A,1}^{(\xi)} \equiv \frac{iL}{I_0} \left(\ln \left(\frac{1}{1 + (\alpha + \alpha_\xi) \cos \theta} \frac{2L}{R} \right) \sin \theta \left\{ \frac{\partial}{\partial \alpha_\xi} + \frac{1 + 2(\alpha + \alpha_\xi) \cos \theta}{2[1 + (\alpha + \alpha_\xi) \cos \theta](\alpha + \alpha_\xi)} \right\} - \frac{1}{4} \frac{\sin(2\theta)}{1 + (\alpha + \alpha_\xi) \cos \theta} \right), \quad (\text{B1c})$$

$$\tilde{\mathcal{H}}_{A,2}^{(\xi)} \equiv \frac{I^2}{4I_0^2} \ln^2 \left\{ \frac{2L}{R[1 + (\alpha + \alpha_\xi) \cos \theta]} \right\} \sin^2 \theta. \quad (\text{B1d})$$

We can observe that the matrix elements of $\tilde{\mathcal{H}}_{\mathbf{A}}^{(2D)}$ and $\tilde{\mathcal{H}}_{\mathbf{A}}^{\xi}$ can only be of the order $\alpha_{\xi_{\max}}^{-1}$ or higher (concrete calculations will show that they actually are of the order $\alpha_{\xi_{\max}}^0$ or higher), so, considering Eq. (16), we obtain

$$\lim_{\alpha_{\xi_{\max}} \rightarrow 0} \frac{\langle \tilde{\mathcal{F}}_{n_2-n,m,k}^{(\Lambda)} | \tilde{\mathcal{H}}_{\mathbf{A}}^{(2D)} | \tilde{\mathcal{F}}_{n_2,m,k}^{(\Lambda)} \rangle}{\langle \tilde{\mathcal{F}}_{n_2,m,1}^{(\Lambda)} | \tilde{\mathcal{H}}_{\text{free}}^{(\xi)} | \tilde{\mathcal{F}}_{n_2,m,1}^{(\Lambda)} \rangle} = \lim_{\alpha_{\xi_{\max}} \rightarrow 0} \frac{\langle \tilde{\mathcal{F}}_{n_2-n,m,k}^{(\Lambda)} | \tilde{\mathcal{H}}_{\mathbf{A}}^{(\xi)} | \tilde{\mathcal{F}}_{n_2,m,k'}^{(\Lambda)} \rangle}{\langle \tilde{\mathcal{F}}_{n_2,m,1}^{(\Lambda)} | \tilde{\mathcal{H}}_{\text{free}}^{(\xi)} | \tilde{\mathcal{F}}_{n_2,m,1}^{(\Lambda)} \rangle} = 0, \quad (\text{B2})$$

for any n_2, n , and m . Equations (15) and (B2) imply that in the limit $\alpha_{\xi_{\max}} \rightarrow 0$ all the matrix elements of $\tilde{\mathcal{H}} - \tilde{\mathcal{H}}_{\text{free}}^{(\xi)}$ are negligible in comparison to $\langle \tilde{\mathcal{F}}_{n_2,m,k}^{(\Lambda)} | \tilde{\mathcal{H}}_{\text{free}}^{(\xi)} | \tilde{\mathcal{F}}_{n_2,m,k'}^{(\Lambda)} \rangle$, for any (finite) n_2, m , and k . Therefore, $\tilde{\mathcal{H}}_{\text{free}}^{(\xi)}$ contributes only the additive constant $\pi^2/\alpha_{\xi_{\max}}^2$ (divergent in the limit $\alpha_{\xi_{\max}} \rightarrow 0$) to the total energy of the system and fixes $k = k' = 1$ —that is, the lowest energy level in the direction ξ . Using this observation, we may calculate the matrix elements of $\tilde{\mathcal{H}}_{\mathbf{A},1}^{(2D)}$ and $\tilde{\mathcal{H}}_{\mathbf{A},2}^{(2D)}$. After integrating over $\alpha_{\xi}, \phi, \theta$, and taking again only the lowest order in $\alpha_{\xi_{\max}}$, we obtain

$$\begin{aligned} \langle \tilde{\mathcal{F}}_{n_2-n,m,1}^{(\Lambda)} | \tilde{\mathcal{H}}_{\mathbf{A},1}^{(2D)} | \tilde{\mathcal{F}}_{n_2,m',1}^{(\Lambda)} \rangle &= \delta_{mm'} \frac{Ia}{I_0} \left[n_2 \left(\frac{I_{n+1}^{(\ln)}(a) + I_{n-1}^{(\ln)}(a)}{2} - \ln \left(\frac{2aL}{R} \right) \frac{\delta_{n+1} + \delta_{n-1}}{2} \right) \right. \\ &\quad \left. + \frac{I_{n+1}^{(\ln)}(a) - I_{n-1}^{(\ln)}(a)}{4} - \ln \left(\frac{2aL}{R} \right) \frac{\delta_{n+1} - \delta_{n-1}}{4} + \frac{I_{n+2}(a) - I_{n-2}(a)}{8} \right], \end{aligned} \quad (\text{B3})$$

where

$$\begin{cases} I_n(a) & \equiv \frac{1}{2\pi} \int_0^{2\pi} e^{in\theta} / (a + \cos \theta) d\theta = \frac{(-a + \sqrt{a^2 - 1})^{|n|}}{\sqrt{a^2 - 1}}, \\ I_n^{(\ln)}(a) & \equiv \frac{1}{2\pi} \int_0^{2\pi} e^{in\theta} \ln(a + \cos \theta) d\theta = \ln \left(\frac{a + \sqrt{a^2 - 1}}{2} \right)_{n=0} - \frac{(-a + \sqrt{a^2 - 1})^{|n|}}{|n|} \Big|_{n \neq 0} \end{cases} \quad (\text{B4})$$

[see the proof of the first Eq. (B4)]. Plugging the Eq. (B4) into Eq. (B3), we get

$$\begin{aligned} \langle \tilde{\mathcal{F}}_{n_2-n,m,1}^{(\Lambda)} | \tilde{\mathcal{H}}_{\mathbf{A},1}^{(2D)} | \tilde{\mathcal{F}}_{n_2,m',1}^{(\Lambda)} \rangle &= \delta_{mm'} \frac{Ia}{I_0} \frac{2n_2 - n}{2} \left\{ (a - \sqrt{a^2 - 1})_{n=0} - \frac{1}{2} \left[\ln \left(\frac{4aL}{R(a + \sqrt{a^2 - 1})} \right) + \frac{(-a + \sqrt{a^2 - 1})^2}{2} \right]_{|n|=1} \right. \\ &\quad \left. + (-a + \sqrt{a^2 - 1})^{|n|} \frac{(a|n| + \sqrt{a^2 - 1})}{(n^2 - 1)} \Big|_{|n|>1} \right\}. \end{aligned} \quad (\text{B5})$$

From Eq. (B1), we obtain

$$\begin{aligned} \langle \tilde{\mathcal{F}}_{n_2-n,m,1}^{(\Lambda)} | \tilde{\mathcal{H}}_{\mathbf{A},1}^{(\xi)} | \tilde{\mathcal{F}}_{n_2,m',1}^{(\Lambda)} \rangle &= \frac{\delta_{mm'}}{2} \left\{ \frac{1}{\alpha_{\xi_{\max}}} \int_0^1 dx \sin(2\pi x) \int_0^{2\pi} d\theta e^{in\theta} \sin \theta \ln \left[\frac{1}{1 + (\alpha + x\alpha_{\xi_{\max}}) \cos \theta} \frac{2L}{R} \right] \right. \\ &\quad \left. - \frac{1}{2\pi} \int_0^1 dx \sin^2(\pi x) \int_0^{2\pi} d\theta \frac{e^{in\theta} \sin(2\theta)}{1 + (\alpha + x\alpha_{\xi_{\max}}) \cos \theta} \right\}. \end{aligned} \quad (\text{B6})$$

Expanding the integrands in Taylor series and keeping only the terms proportional to $\alpha_{\xi_{\max}}^{-1}$ and $\alpha_{\xi_{\max}}^0$ (which remain different from zero in the limit $\alpha_{\xi_{\max}} \rightarrow 0$), upon integration over x we obtain

$$\langle \tilde{\mathcal{F}}_{n_2-n,m,1}^{(\Lambda)} | \tilde{\mathcal{H}}_{\mathbf{A},1}^{(\xi)} | \tilde{\mathcal{F}}_{n_2,m',1}^{(\Lambda)} \rangle = 0. \quad (\text{B7})$$

For the two remaining terms, we have

$$\begin{aligned} \langle \tilde{\mathcal{F}}_{n_2-n,m,k}^{(\Lambda)} | \tilde{\mathcal{H}}_{\mathbf{A},2}^{(2D)} | \tilde{\mathcal{F}}_{n_2,m',k'}^{(\Lambda)} \rangle &= \delta_{mm'} \delta_{kk'} \frac{I^2}{16I_0^2} \left\{ \ln \left(\frac{2aL}{R} \right)^2 (\delta_{n+2} + 2\delta_n + \delta_{n-2}) - 2 \ln \left(\frac{2aL}{R} \right) [I_{n+2}^{(\ln)}(a) + 2I_n^{(\ln)}(a) + I_{n-2}^{(\ln)}(a)] \right. \\ &\quad \left. + [I_{n+2}^{(\ln^2)}(a) + 2I_n^{(\ln^2)}(a) + I_{n-2}^{(\ln^2)}(a)] \right\}, \end{aligned} \quad (\text{B8a})$$

$$\begin{aligned} \langle \tilde{\mathcal{F}}_{n_2-n,m,k}^{(\Lambda)} | \tilde{\mathcal{H}}_{\mathbf{A},2}^{(\xi)} | \tilde{\mathcal{F}}_{n_2,m',k'}^{(\Lambda)} \rangle &= \delta_{mm'} \delta_{kk'} \frac{I^2}{16I_0^2} \left\{ \ln \left(\frac{2aL}{R} \right)^2 (-\delta_{n+2} + 2\delta_n - \delta_{n-2}) - 2 \ln \left(\frac{2aL}{R} \right) [-I_{n+2}^{(\ln)}(a) + 2I_n^{(\ln)}(a) - I_{n-2}^{(\ln)}(a)] \right. \\ &\quad \left. + [-I_{n+2}^{(\ln^2)}(a) + 2I_n^{(\ln^2)}(a) - I_{n-2}^{(\ln^2)}(a)] \right\}, \end{aligned} \quad (\text{B8b})$$

where (see Appendix F)

$$I_n^{(\ln^2)}(a) \equiv \frac{1}{2\pi} \int_0^{2\pi} e^{in\theta} \ln^2(a + \cos \theta) d\theta, \quad \text{with} \quad I_n^{(\ln^2)}(a) \stackrel{a \gg 1}{\sim} \ln^2 a \delta_{n,0} + \frac{\ln a}{a} \delta_{|n|,1} + \frac{(1 - \ln a)}{4a^2} (\delta_{|n|,2} + 2\delta_{n,0}). \quad (\text{B9})$$

Plugging Eqs. (B4) and (B9) into Eq. (B8), we obtain

$$\begin{aligned} \langle \tilde{\mathcal{F}}_{n_2-n,m,1}^\Lambda | \tilde{\mathcal{H}}_{\Lambda,2}^{(2D)} | \tilde{\mathcal{F}}_{n_2,m,1}^\Lambda \rangle = & \frac{I^2}{8I_0^2} \left[\ln \left(\frac{2aL}{R} \right) \left(\left\{ \ln \left[\frac{8aL}{R(a + \sqrt{a^2 - 1})^2} \right] + (-a + \sqrt{a^2 - 1})^2 \right\}_{n=0} \right. \right. \\ & + \left. \left. \frac{(-a + \sqrt{a^2 - 1})[(-a + \sqrt{a^2 - 1})^2 + 9]}{3} \right|_{|n|=1} + \frac{1}{2} \left\{ \ln \left[\frac{8aL}{R(a + \sqrt{a^2 - 1})^2} \right] \right. \right. \\ & + \left. \left. \frac{[(-a + \sqrt{a^2 - 1})^2 + 4]}{2} (-a + \sqrt{a^2 - 1})^2 \right\}_{|n|=2} \right. \\ & \left. \left. + \frac{4(-a + \sqrt{a^2 - 1})^{|n|} [a^2 n^2 + 2a|n|\sqrt{a^2 - 1} - 2]}{|n|(n^2 - 4)} \right|_{|n|>2} \right) + \tilde{I}_n^{(\ln^2, +)}(a) \right], \quad (\text{B10a}) \end{aligned}$$

$$\begin{aligned} \langle \tilde{\mathcal{F}}_{n_2-n,m,1}^\Lambda | \tilde{\mathcal{H}}_{\Lambda,2}^{(\xi)} | \tilde{\mathcal{F}}_{n_2,m,1}^\Lambda \rangle = & \frac{I^2}{8I_0^2} \left[-\ln \left(\frac{2aL}{R} \right) \left(-\left\{ \ln \left[\frac{8aL}{R(a + \sqrt{a^2 - 1})^2} \right] - (-a + \sqrt{a^2 - 1})^2 \right\}_{n=0} \right. \right. \\ & + \left. \left. \frac{2(-a + \sqrt{a^2 - 1})^2(a + 2\sqrt{a^2 - 1})}{3} \right|_{|n|=1} + \frac{1}{2} \left\{ \ln \left[\frac{8aL}{R(a + \sqrt{a^2 - 1})^2} \right] + \frac{(3a + 5\sqrt{a^2 - 1})}{2} \right. \right. \\ & \left. \left. \times (-a + \sqrt{a^2 - 1})^3 \right\}_{|n|=2} + \frac{4(-a + \sqrt{a^2 - 1})^{|n|} [(a^2 - 1)n^2 + 2a|n|\sqrt{a^2 - 1} + 2]}{|n|(n^2 - 4)} \right|_{|n|>2} \right) \\ & \left. + \tilde{I}_n^{(\ln^2, -)}(a) \right], \quad (\text{B10b}) \end{aligned}$$

where

$$\begin{aligned} \tilde{I}_n^{(\ln^2, \pm)}(a) \equiv & \frac{1}{2\pi} \int_0^{2\pi} e^{in\theta} [1 \pm \cos(2\theta)] \ln^2(a + \cos \theta) d\theta, \quad \text{with} \quad \tilde{I}_n^{(\ln^2, \pm)}(1) = \text{finite for any integer } n \text{ and} \\ \tilde{I}_n^{(\ln^2, \pm)}(a) \stackrel{a \gg 1}{\sim} & \ln^2 a \left(\delta_{n,0} \pm \frac{\delta_{|n|,2}}{2} \right) + \frac{\ln a}{a} \left[\left(1 \pm \frac{1}{2} \right) \delta_{|n|,1} \pm \frac{\delta_{|n|,3}}{2} \right] + \frac{(1 - \ln a)}{4a^2} \left[(2 \pm 1) \delta_{n,0} + (1 \pm 1) \delta_{|n|,2} \pm \frac{\delta_{|n|,4}}{2} \right]. \quad (\text{B10c}) \end{aligned}$$

Adding Eq. (B10) and using the definitions (A3), we obtain

$$\begin{aligned} \langle \tilde{\mathcal{F}}_{n_2-n,m,1}^{(\Lambda)} | \tilde{\mathcal{H}}_{\Lambda,2}^{(2D)} + \tilde{\mathcal{H}}_{\Lambda,2}^{(\xi)} | \tilde{\mathcal{F}}_{n_2,m,1}^{(\Lambda)} \rangle \\ = \frac{I^2}{4I_0^2} \left\{ \ln \left(\frac{2aL}{R} \right) \ln \left[\frac{8aL}{R(a + \sqrt{a^2 - 1})^2} \right]_{n=0} + 2 \ln \left(\frac{2aL}{R} \right) \frac{(-a + \sqrt{a^2 - 1})^{|n|}}{|n|} \right|_{n \neq 0} + I_n^{(\ln^2)}(a) \right\}. \quad (\text{B11}) \end{aligned}$$

Figure 9 illustrates the behavior of the functions $\tilde{I}_n^{(\ln^2, -)}(a)$. Panel (a) represents $\tilde{I}_n^{(\ln^2, -)}(1)$ versus n for $n = 1, \dots, 30$, showing a rapid decrease in magnitude as n increases. Panel (b) represents $\tilde{I}_n^{(\ln^2, \pm)}(a)$ versus a for $n = 0, \dots, 4$ (solid lines), demonstrating a quick convergence to their asymptotic approximations from Eq. (B10c) (dash-dot lines). These empirical results are explained by the analytical behavior for large a . According to Eq. (B10c), the approximations for $\tilde{I}_0^{(\ln^2, \pm)}(a)$ and $\tilde{I}_2^{(\ln^2, \pm)}(a)$ are dominated by terms proportional to $\ln^2 a$, while for $n \neq 0, 2$, the leading term scales as $\ln a/a^n$. This dependence on $1/a^n$ accounts for a sharp decay of $|\tilde{I}_n^{(\ln^2, -)}(a)|$ with increasing values of both n and a .

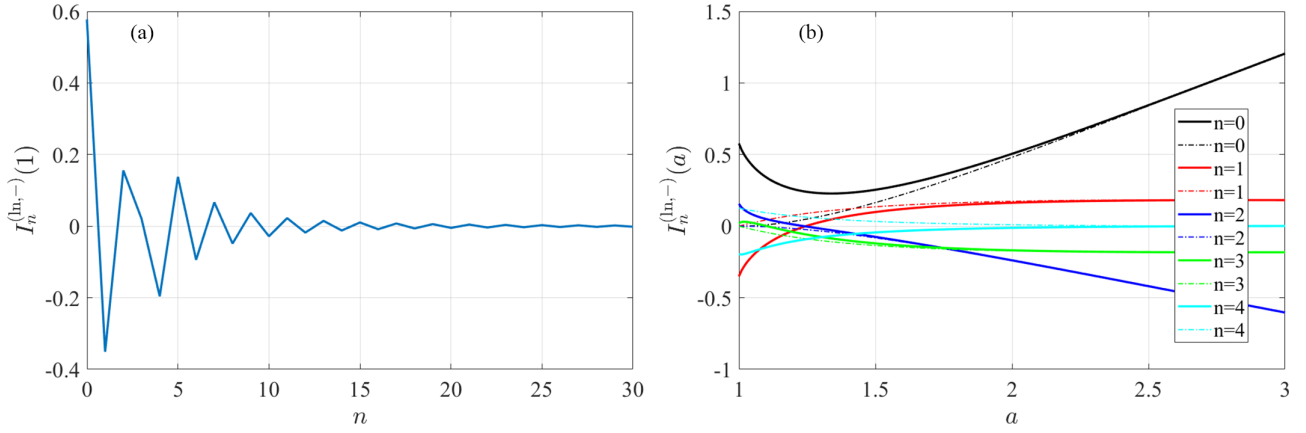


FIG. 9. (a) The function $\tilde{I}_n^{(\ln, -)}(1)$ vs n and (b) $\tilde{I}_n^{(\ln, -)}(a)$ vs a , for the values $n = -4, \dots, 4$, as indicated in the legend. We observe that the asymptotic values are very rapidly approached as a increases. The asymptotic expressions for $n = -4, \dots, 4$ are given in Eq. (B10c) and for larger values of $|n|$ are given in Eq. (F6).

2. The matrix elements of the toroidal dipole

Using again Taylor expansions in $\alpha_{\xi_{\max}}$, from the expressions of Sec. II B and Appendix A 2, we obtain in the lowest order

$$\langle \mathcal{F}_{n_2-n, m, 1}^{(\Lambda)} | \tilde{T}_{3,0}^{(\theta)} | \mathcal{F}_{n_2, m', 1}^{(\Lambda)} \rangle = \delta_{mm'} \left\{ -\frac{3}{4} \left(n_2 + \frac{n}{4} \right) \Big|_{|n|=2} - \frac{1}{a} \left[n_2(a^2 + 1) - \frac{n(a^2 - 2)}{4} \right] \Big|_{|n|=1} - \frac{5n_2}{2} \delta_n + \text{sgn}(n) \frac{(a^2 - 1)(-a + \sqrt{a^2 - 1})^{|n|}}{2} \right\}, \quad (\text{B12a})$$

$$\langle \mathcal{F}_{n_2-n, m, 1}^{(\Lambda)} | \tilde{T}_{3,0}^{(\xi)} | \mathcal{F}_{n_2, m', 1}^{(\Lambda)} \rangle = \delta_{mm'} \left\{ \frac{9n}{16} \Big|_{|n|=2} + \frac{n(a^2 + 4)}{4a} \Big|_{|n|=1} - \frac{\text{sgn}(n)(a^2 - 1)(-a + \sqrt{a^2 - 1})^{|n|}}{2} \right\}, \quad (\text{B12b})$$

$$\langle \mathcal{F}_{n_2-n, m, 1}^{(\Lambda)} | \tilde{T}_{3,A}^{(\theta)} | \mathcal{F}_{n_2, m', 1}^{(\Lambda)} \rangle = \frac{\delta_{mm'}}{2a^2} \frac{I}{I_0} \left\{ \ln \left(\frac{2aL}{R} \right) \left[\frac{3a}{4} \frac{\delta_{n+3} + \delta_{n-3}}{2} + (a^2 + 1) \frac{\delta_{n+2} + \delta_{n-2}}{2} + \frac{13a}{4} \frac{\delta_{n+1} + \delta_{n-1}}{2} + (a^2 + 1) \delta_n \right] - \frac{3a}{4} \frac{I_{n+3}^{(\ln)}(a) + I_{n-3}^{(\ln)}(a)}{2} - (a^2 + 1) \frac{I_{n+2}^{(\ln)}(a) + I_{n-2}^{(\ln)}(a)}{2} - \frac{13a}{4} \frac{I_{n+1}^{(\ln)}(a) + I_{n-1}^{(\ln)}(a)}{2} - (a^2 + 1) I_n^{(\ln)}(a) \right\}, \quad (\text{B12c})$$

$$\langle \mathcal{F}_{n_2-n, m, 1}^{(\Lambda)} | \tilde{T}_{3,A}^{(\xi)} | \mathcal{F}_{n_2, m', 1}^{(\Lambda)} \rangle = \frac{\delta_{mm'}}{18a^2} \frac{I}{I_0} \left(\ln \left(\frac{2aL}{R} \right) [4(1 + 2a^2)\delta_n + 3a(\delta_{n+1} + \delta_{n-1}) - 2(1 + 2a^2)(\delta_{n+2} + \delta_{n-2}) - 3a(\delta_{n+3} + \delta_{n-3})] - \{4(1 + 2a^2)I_n^{(\ln)}(a) + 3a[I_{n+1}^{(\ln)}(a) + I_{n-1}^{(\ln)}(a)] - 2(1 + 2a^2)[I_{n+2}^{(\ln)}(a) + I_{n-2}^{(\ln)}(a)] - 3a[I_{n+3}^{(\ln)}(a) + I_{n-3}^{(\ln)}(a)] \} \right). \quad (\text{B12d})$$

Using Eq. (B4), we get

$$\begin{aligned} & \langle \mathcal{F}_{n_2-n, m, 1}^{(\Lambda)} | \tilde{T}_{3,A}^{(\theta)} | \mathcal{F}_{n_2, m', 1}^{(\Lambda)} \rangle \\ &= \frac{\delta_{mm'}}{2a^2} \frac{I}{I_0} \left\{ \left((a^2 + 1) \ln \left[\frac{4aL}{R(a + \sqrt{a^2 - 1})} \right] - 2a(a - \sqrt{a^2 - 1}) - \frac{1}{2} \right) \Big|_{n=0} \right. \\ &+ \left\{ \frac{13a}{8} \ln \left[\frac{4aL}{R(a + \sqrt{a^2 - 1})} \right] + \left(-\frac{1}{12}a^4 + \frac{3}{8}a^2 + \frac{4}{3} \right) \sqrt{a^2 - 1} + \frac{a^5}{12} - \frac{5a^3}{12} - \frac{61a}{32} \right\} \Big|_{|n|=1} \\ &+ \left\{ \frac{(a^2 + 1)}{2} \ln \left[\frac{4aL}{R(a + \sqrt{a^2 - 1})} \right] + \frac{(-a + \sqrt{a^2 - 1})^3}{8} \left[\left(\frac{139a^2}{5} - 3 \right) \sqrt{a^2 - 1} + \frac{a}{5} \left(141a^2 - \frac{259}{3} \right) \right] \right\} \Big|_{|n|=2} \end{aligned}$$

$$\begin{aligned}
 & + \left\{ \frac{3a}{8} \ln \left[\frac{4aL}{R(a + \sqrt{a^2 - 1})} \right] + \frac{(-a + \sqrt{a^2 - 1})^3}{5} \left[\frac{(168a^3 + 53a)\sqrt{a^2 - 1}}{32} + \frac{19a^4}{4} - \frac{47a^2}{96} - \frac{4}{3} \right] \right\}_{|n|=3} \\
 & - \frac{(-a + \sqrt{a^2 - 1})^{|n|}}{|n|(n^2 - 1)(n^2 - 4)(n^2 - 9)} \left\{ a\sqrt{a^2 - 1} [(5a^2 - 3)n^4 - (5a^2 - 9)n^2 + 72]|n| \right. \\
 & \left. + a^2(a^2 - 1)n^6 + (5a^4 - 7a^2 + 4)n^4 - 2(3a^4 - 25a^2 + 20)n^2 + 36a^2 + 36 \right\}_{|n|>3} \Bigg), \tag{B13a}
 \end{aligned}$$

$$\begin{aligned}
 & \langle \mathcal{F}_{n_2-n, m, 1}^{(\Lambda)} | \tilde{T}_{3, \mathbf{A}}^{(\xi)} | \mathcal{F}_{n_2, m', 1}^{(\Lambda)} \rangle \\
 & = \frac{\delta_{mm'}}{2a^2} \frac{I}{I_0} \left(\left\{ \frac{(1 + 2a^2)}{2} \ln \left[\frac{4aL}{R(a + \sqrt{a^2 - 1})} \right] + \frac{3a(-a + \sqrt{a^2 - 1})}{2} + \frac{1}{4} \right\}_{n=0} \right. \\
 & + \left\{ \frac{3a}{8} \ln \left[\frac{4aL}{R(a + \sqrt{a^2 - 1})} \right] + \frac{(2a^4 - a^2 + 8)(-a + \sqrt{a^2 - 1})}{24} + \frac{a^3}{24} - \frac{25a}{96} \right\}_{|n|=1} \\
 & + \left\{ -\frac{(1 + 2a^2)}{4} \ln \left[\frac{4aL}{R(a + \sqrt{a^2 - 1})} \right] - \frac{a(4a^4 - 8a^2 + 19)(-a + \sqrt{a^2 - 1})}{20} - \frac{a^4}{10} + \frac{7a^2}{40} - \frac{5}{16} \right\}_{|n|=2} \\
 & + \left\{ -\frac{3a}{8} \ln \left[\frac{4aL}{R(a + \sqrt{a^2 - 1})} \right] - (-a + \sqrt{a^2 - 1})^3 \left[\frac{a(168a^2 + 69)\sqrt{a^2 - 1}}{160} + \frac{19a^4}{20} + \frac{13a^2}{96} - \frac{7}{15} \right] \right\}_{|n|=3} \\
 & + \frac{(-a + \sqrt{a^2 - 1})^{|n|}}{|n|(n^2 - 1)(n^2 - 2)(n^2 - 3)} \left\{ (a^2 - 1)^2 n^6 + 5a(a^2 - 1)\sqrt{a^2 - 1} |n|^5 + (a^2 - 1)(5a^2 + 12)n^4 \right. \\
 & \left. - a(5a^2 - 41)\sqrt{a^2 - 1} |n|^3 - (6a^4 - 13a^2 - 29)n^2 - 54\sqrt{a^2 - 1} a |n| - 18(2a^2 - 1) \right\}_{|n|>3} \Bigg). \tag{B13b}
 \end{aligned}$$

It is interesting to note that both Eqs. (B12a) and (B12b) do not form hermitian matrices and this happens because $\tilde{T}_{3,0}^{(\theta)}$ and $\tilde{T}_{3,0}^{(\xi)}$ are not hermitian operators. Moreover, while $\tilde{T}_{3,0}^{(\xi)}$ has matrix elements which are antisymmetric in n , whereas the sum $\tilde{T}_{3,0}^{(\theta)} + \tilde{T}_{3,0}^{(\xi)}$ is hermitian, we have the relations

$$\begin{aligned}
 & \langle \mathcal{F}_{n_2-n, m, 1}^{(\Lambda)} | \tilde{T}_{3,0}^{(\xi)} | \mathcal{F}_{n_2, m', 1}^{(\Lambda)} \rangle = -\langle \mathcal{F}_{n_2, m, 1}^{(\Lambda)} | \tilde{T}_{3,0}^{(\xi)} | \mathcal{F}_{n_2-n, m', 1}^{(\Lambda)} \rangle, \tag{B14a} \\
 & \langle \mathcal{F}_{n_2-n, m, 1}^{(\Lambda)} | \tilde{T}_{3,0}^{(\xi)} + \tilde{T}_{3,0}^{(\theta)} | \mathcal{F}_{n_2, m', 1}^{(\Lambda)} \rangle = -\delta_{mm'} \left[\frac{3(2n_2 - n)}{8} \Big|_{|n|=2} + \frac{(a^2 + 1)(2n_2 - n)}{2a} \Big|_{|n|=1} + \frac{5n_2}{2} \Big|_{n=0} \right] \\
 & = \langle \mathcal{F}_{n_2-n, m, 1}^{(\Lambda)} | \tilde{T}_3^{(\theta)} (I = 0) | \mathcal{F}_{n_2, m', 1}^{(\Lambda)} \rangle = \langle \mathcal{F}_{n_2-n, m, 1}^{(\Lambda)} | \tilde{T}_{3,0}^{(\theta)} | \mathcal{F}_{n_2, m', 1}^{(\Lambda)} \rangle + \langle \mathcal{F}_{n_2, m, 1}^{(\Lambda)} | \tilde{T}_{3,0}^{(\theta)} | \mathcal{F}_{n_2-n, m', 1}^{(\Lambda)} \rangle, \tag{B14b}
 \end{aligned}$$

where $\tilde{T}_3^{(\theta)} (I = 0) \equiv \tilde{T}_{3,0}^{(\theta)} - \tilde{T}_\theta$ (A5) is the toroidal dipole at $\mathbf{A} = 0$ [10].

From Eqs. (B12) and (B13), we have

$$\begin{aligned}
 & \langle \mathcal{F}_{n_2-n, m, 1}^{(\Lambda)} | \tilde{T}_{3, \mathbf{A}}^{(\theta)} + \tilde{T}_{3, \mathbf{A}}^{(\xi)} | \mathcal{F}_{n_2, m', 1}^{(\Lambda)} \rangle \\
 & = \delta_{mm'} \frac{I}{2a^2 I_0} \left\{ \ln \left(\frac{2aL}{R} \right) \left[\frac{\delta_{n+2} + \delta_{n-2}}{4} + 2a(\delta_{n+1} + \delta_{n-1}) + \frac{3 + 4a^2}{2} \delta_n \right] \right. \\
 & \left. - \left[\frac{I_{n+2}^{(\text{ln})}(a) + I_{n-2}^{(\text{ln})}(a)}{4} + 2a(I_{n+1}^{(\text{ln})}(a) + I_{n-1}^{(\text{ln})}(a)) + \frac{3 + 4a^2}{2} I_n^{(\text{ln})}(a) \right] \right\} \\
 & = \delta_{mm'} \frac{I}{2a^2 I_0} \left(\frac{1}{4} \left\{ \ln \left[\frac{4aL}{R(a + \sqrt{a^2 - 1})} \right] + \frac{(-a + \sqrt{a^2 - 1})^2 (-74a^2 + 33 - 70a\sqrt{a^2 - 1})}{12} \right\}_{|n|=2} \right. \\
 & \left. + \left\{ 2a \ln \left[\frac{4aL}{R(a + \sqrt{a^2 - 1})} \right] + \frac{(-a + \sqrt{a^2 - 1})(7a^2 + 10 + 5a\sqrt{a^2 - 1})}{6} \right\}_{|n|=1} \right)
 \end{aligned}$$

$$+ \left\{ \frac{3 + 4a^2}{2} \ln \left[\frac{4aL}{R(a + \sqrt{a^2 - 1})} \right] + \frac{(-a + \sqrt{a^2 - 1})(15a + \sqrt{a^2 - 1})}{4} \right\}_{n=0} \\ + (-a + \sqrt{a^2 - 1})^{|n|} \left\{ \frac{-(a^2 - 1)n^4 - 2a\sqrt{a^2 - 1}|n|^3 + (5a^2 - 7)n^2 + 14a\sqrt{a^2 - 1}|n| + 8a^2 + 6}{|n|(n^2 - 1)(n^2 - 4)} \right\}_{|n|>2}. \quad (\text{B15})$$

APPENDIX C: ABRUPT CHANGES OF $\langle \tilde{T}_3^{(\theta)}(I) \rangle_{l,m,1}$ AROUND INTEGER AND HALF-INTEGER VALUES OF I/I_{per}

We show now that $\langle \tilde{T}_3^{(\theta)}(I) \rangle_{l,m,1}$ (29) has abrupt changes around $I/I_{\text{per}} = \eta/2$, where η is an integer. For this, let us fix a sufficiently large excitation level l , such that Eq. (25) applies for our arguments, and a positive integer η ; for clarity, let us assume that l is even and $0 \leq \eta < l/2$. Then, we define the integers $n_2 \equiv l/2 - \eta > 0$ and $n'_2 \equiv -l/2 - \eta < 0$, such that

$$l = 2(n_2 + \eta) \equiv 2n_2^{(I)}|_{n_2=l/2-\eta, I=\eta I_{\text{per}}} = 2(-n'_2 - \eta) \\ = 2|n'_2 + \eta| \equiv 2|n_2^{(I)}|_{n_2=-(l/2+\eta), I=\eta I_{\text{per}}}. \quad (\text{C1})$$

If we choose I so that $\eta \leq I/I_{\text{per}} < \eta + 0.5$ (that is, $[I/I_{\text{per}}] = \eta$), then, according to Eq. (28) and the definition (C1), $n_2^{(I)}|_{n_2=l/2-\eta}$ corresponds to the level l (notice that $l/2 \leq n_2^{(I)}|_{n_2=l/2-\eta} \equiv l/2 - \eta + I/I_{\text{per}} < l/2 + 0.5$), whereas $(n'_2)^{(I)}|_{n'_2=-l/2-\eta}$ corresponds to the level $l-1$ (notice that $-l/2 + 0.5 > (n'_2)^{(I)}|_{n'_2=-l/2-\eta, I} \equiv -l/2 - \eta + I/I_{\text{per}} \geq -l/2$). On the other hand, if $\eta - 0.5 \leq I/I_{\text{per}} < \eta$ (again, $[I/I_{\text{per}}] = \eta$), then $n_2^{(I)}|_{n_2=l/2-\eta}$ ($l/2 - 0.5 \leq n_2^{(I)}|_{n_2=l/2-\eta} \equiv l/2 - \eta + I/I_{\text{per}} < l/2$) corresponds to the level $l-1$ (C1), whereas $(n'_2)^{(I)}|_{n'_2=-l/2-\eta}$ corresponds to the level l [since $-l/2 > (n'_2)^{(I)}|_{n'_2=-l/2-\eta, I} \equiv -l/2 - \eta + I/I_{\text{per}} \geq -l/2 - 0.5$]. Therefore, with increasing current, around $I = \eta I_{\text{per}}$, the level l , defined by Eq. (C1), switches from the transformed quantum number $(n'_2)^{(I)}|_{n'_2=-l/2-\eta, I=\eta I_{\text{per}}} \equiv -l/2$ to $n_2^{(I)}|_{n_2=l/2-\eta, I=\eta I_{\text{per}}} = l/2$, whereas the level $l-1$ switches from the transformed quantum number $n_2^{(I)}|_{n_2=l/2-\eta, I=\eta I_{\text{per}}} \equiv l/2$ to $(n'_2)^{(I)}|_{n'_2=-l/2-\eta, I=\eta I_{\text{per}}} \equiv -l/2$. This implies that the expectation value $\langle \tilde{T}_3^{(\theta)}(I) \rangle_{l,m,1}$ changes from $2.5(l/2)$ to $-2.5(l/2)$, whereas $\langle \tilde{T}_3^{(\theta)}(I) \rangle_{l-1,m,1}$ changes from $-2.5(l/2)$ to $2.5(l/2)$, as observed in Fig. 4.

Now, we apply a similar argument for the interval $\eta + 0.5 \leq I/I_{\text{per}} < \eta + 1$ (that is, $[I/I_{\text{per}}] = \eta + 1$). Then, according to Eqs. (28) and (C1), $n_2^{(I)}|_{n_2=l/2-\eta-1}$ corresponds to the level $l-1$ (since $l/2 - 0.5 \leq n_2^{(I)}|_{n_2=l/2-\eta-1} \equiv l/2 - \eta - 1 + I/I_{\text{per}} < l/2$), whereas

$(n'_2)^{(I)}|_{n'_2=-l/2-\eta-1}$ corresponds to the level l [since $-l/2 > (n'_2)^{(I)}|_{n'_2=-l/2-\eta-1} \equiv -l/2 - \eta - 1 + I/I_{\text{per}} \geq -l/2 - 0.5$]. Therefore, as the current increases, around $I = (\eta + 0.5)I_{\text{per}}$, the level l switches from the transformed quantum number $n_2^{(I)}|_{n_2=l/2-\eta, I=(\eta+0.5)I_{\text{per}}} = l/2 + 0.5$ to $(n'_2)^{(I)}|_{n'_2=-l/2-\eta-1, I=(\eta+0.5)I_{\text{per}}} = -l/2 - 0.5$, whereas the level $l-1$ switches from the transformed quantum number $(n'_2)^{(I)}|_{n'_2=-l/2-\eta, I=(\eta+0.5)I_{\text{per}}} = -l/2 + 0.5$ to $n_2^{(I)}|_{n_2=l/2-\eta-1, I=(\eta+0.5)I_{\text{per}}} \equiv l/2 - 0.5$. This implies that $\langle \tilde{T}_3^{(\theta)}(I) \rangle_{l,m,1}$ changes from $-2.5(l/2 + 0.5)$ to $2.5(l/2 - 0.5)$, whereas $\langle \tilde{T}_3^{(\theta)}(I) \rangle_{l-1,m,1}$ changes from $2.5(l/2 - 0.5)$ to $-2.5(l/2 - 0.5)$, as also observed in Fig. 4.

These abrupt changes may also be observed in the simulations of Table I [18]. In these simulations we see the change of the Hamiltonian eigenvectors as the current is gradually increased. If, at low current, but high enough energy level or a , the vectors of the basis [Eq. (14a) or (23)] are good approximations for the energy eigenvectors, as I increases, more and more basis vectors start to significantly contribute to the eigenvectors. This may seem to be in contradiction with our observations of Sec. III D, where we approximate the eigenvectors transformed by $\mathcal{U}$ (7) by the vectors of the transformed basis [Eq. (23)]. However, for example, $\tilde{\mathcal{F}}_{n_2^{(I)}, m, k}^{(\Lambda)}(\theta, \phi, \alpha_\xi)$ (23) is an approximation for the eigenvector corresponding to the energy $\tilde{E}_{n_2^{(I)}, m, 1}^{(2D)}$ (25), and this corresponds, in the original Hilbert space, to $\mathcal{U}^{-1} \tilde{\mathcal{F}}_{n_2^{(I)}, m, k}^{(\Lambda)}(\theta, \phi, \alpha_\xi)$, which is not anymore one of the vectors in the basis [Eq. (14a)], so more and more basis vectors significantly contribute to the expansion of the energy eigenfunction, as I increases.

APPENDIX D: THE CONTRIBUTION OF THE ξ DIRECTION TO THE 2D APPROXIMATION

The full effective Hamiltonian is given by Eq. (18), with the matrix elements of $\tilde{\mathcal{H}}_{A,2}^{(\xi)}$ given by Eq. (B10b). To better understand the contribution of $\tilde{\mathcal{H}}_{A,2}^{(\xi)}$ to the energy spectrum, we compare the matrix elements (B10b) with the diagonal elements (15a). Considering that the diagonal elements are proportional to a^2 , for the matrix elements (B10b), we write

$$\langle \tilde{\mathcal{F}}_{n_2-n, m, 1}^\Lambda | \tilde{\mathcal{H}}_{A,2}^{(\xi)} | \tilde{\mathcal{F}}_{n_2, m, 1}^\Lambda \rangle \equiv \frac{I^2}{I_{\text{per}}^2} a^2 \left[\delta_{n,0} h_0 \left(a; \frac{L}{R} \right) + \delta_{|n|,1} h_1 \left(a; \frac{L}{R} \right) + \delta_{|n|,2} h_2 \left(a; \frac{L}{R} \right) + h_3 \left(a, n; \frac{L}{R} \right) \right], \quad (\text{D1a})$$

where

$$h_0 \left(a; \frac{L}{R} \right) \equiv P(a) \left[\ln \left(\frac{2aL}{R} \right) \left\{ \ln \left[\frac{8aL}{R(a + \sqrt{a^2 - 1})^2} \right] - (a - \sqrt{a^2 - 1})^2 \right\} + \tilde{I}_0^{(\ln^2, -)}(a) \right], \quad (\text{D1b})$$

$$h_1\left(a; \frac{L}{R}\right) \equiv P(a) \left[-\ln\left(\frac{2aL}{R}\right) \frac{2(-a + \sqrt{a^2 - 1})^2(a + 2\sqrt{a^2 - 1})}{3} + \tilde{I}_n^{(\ln^2, -)}(a) \right], \quad (\text{D1c})$$

$$h_2\left(a; \frac{L}{R}\right) \equiv P(a) \left[-\ln\left(\frac{2aL}{R}\right) \frac{1}{2} \left\{ \ln\left[\frac{8aL}{R(a + \sqrt{a^2 - 1})^2}\right] - \frac{(3a + 5\sqrt{a^2 - 1})(a - \sqrt{a^2 - 1})^3}{2} \right\} + \tilde{I}_n^{(\ln^2, -)}(a) \right], \quad (\text{D1d})$$

$$h_3\left(a; n; \frac{L}{R}\right) \equiv P(a) \left[-\ln\left(\frac{2aL}{R}\right) \frac{4[(a^2 - 1)n^2 + 2a|n|\sqrt{a^2 - 1} + 2](-a + \sqrt{a^2 - 1})^{|n|}}{|n|(n^2 - 4)} + \tilde{I}_n^{(\ln^2, -)}(a) \right], \text{ if } |n| > 2, \quad (\text{D1e})$$

$$\text{with } P(a) \equiv \frac{1}{2a^2(a - \sqrt{a^2 - 1})^2}, \quad (\text{D1f})$$

are plotted in Fig. 10.

Analyzing the prefactor $P(a)$, we observe that

$$P(1) = \frac{1}{2}, \quad P(a) \stackrel{a \gg 1}{\approx} 2 - \frac{1}{a^2}, \quad \text{whereas } P(a) < 2, \quad \frac{dP(a)}{da} = \frac{1}{\sqrt{a^2 - 1}(a - \sqrt{a^2 - 1})a^3} > 0 \quad \text{for } \forall a > 1. \quad (\text{D2})$$

Further, we have the limiting cases of Eq. (D1):

$$h_0\left(1; \frac{L}{R}\right) = \frac{\delta_{n,0}}{2} \left[\ln\left(\frac{2L}{R}\right) \left\{ \ln\left[\frac{8L}{R}\right] - 1 \right\} + \tilde{I}_0^{(\ln^2, -)}(1) \right], \quad (\text{D3a})$$

$$h_1\left(1; \frac{L}{R}\right) = \frac{\delta_{|n|,1}}{2} \left[-\ln\left(\frac{2L}{R}\right) \frac{2}{3} + \tilde{I}_1^{(\ln^2, -)}(1) \right], \quad (\text{D3b})$$

$$h_2\left(1; \frac{L}{R}\right) = \frac{\delta_{|n|,2}}{2} \left[-\ln\left(\frac{2L}{R}\right) \frac{1}{2} \left\{ \ln\left[\frac{8L}{R}\right] - \frac{3}{2} \right\} + \tilde{I}_2^{(\ln^2, -)}(1) \right], \quad (\text{D3c})$$

$$h_3\left(1; \frac{L}{R}, n\right) = \frac{1}{2} \left[-\ln\left(\frac{2L}{R}\right) \frac{8}{|n|(n^2 - 4)} (-1)^{|n|} + \tilde{I}_n^{(\ln^2, -)}(1) \right], \quad \text{if } |n| > 2, \quad (\text{D3d})$$

with $\tilde{I}_n^{(\ln^2, -)}(1)$ plotted in Fig. 9, and

$$h_0\left(a; \frac{L}{R}\right) \stackrel{a \gg 1}{\approx} \delta_{n,0} \left\{ 2 \ln\left(\frac{2L}{R}\right)^2 + \frac{1}{a^2} \left[-\ln^2\left(\frac{2L}{R}\right) + \frac{1}{2} \ln\left(\frac{2L}{R}\right) + \frac{1}{2} \right] \right\}, \quad (\text{D4a})$$

$$h_1\left(a; \frac{L}{R}\right) \stackrel{a \gg 1}{\approx} \delta_{|n|,1} \left[-\frac{\ln\left(\frac{2L}{R}\right) + \ln(a)}{a} + \frac{2 \ln\left(\frac{2L}{R}\right) - 3 \ln a}{6a^3} \right], \quad (\text{D4b})$$

$$h_2\left(a; \frac{L}{R}\right) \stackrel{a \gg 1}{\approx} -\delta_{|n|,2} \left[\ln^2\left(\frac{2L}{R}\right) - 2 \ln^2(a) \right] \left(1 - \frac{1}{2a^2} \right), \quad (\text{D4c})$$

$$h_3\left(a; \frac{L}{R}, n\right) \stackrel{a \gg 1}{\approx} -\ln\left(\frac{2L}{R}\right) \frac{2(4|n|a^2 + n^2 - 6|n| + 4)}{(|n| - 2)|n|} \left(\frac{-1}{2a}\right)^{|n|} + \tilde{I}_n^{(\ln^2, -)}(1), \quad \text{if } |n| > 2, \quad (\text{D4d})$$

where the expansions for $\tilde{I}_n^{(\ln^2, -)}(a)$ are given in Eq. (B10c) for $|n| \leq 4$ and in Eq. (F6) for $|n| \geq 4$. Obviously, in the limit $a \rightarrow \infty$ only the terms h_0 and h_2 survive, as can be seen also in Fig. 10.

To make sure that $h_3(a; L/R, n)$ does not become significant for certain values of n , from Eq. (D1e) observe that

$$[(a^2 - 1)n^2 + 2a|n|\sqrt{a^2 - 1} + 2] > 0, \quad (\text{D5a})$$

$$\frac{\partial}{\partial n} \left[\frac{4[(a^2 - 1)n^2 + 2a|n|\sqrt{a^2 - 1} + 2]}{|n|(n^2 - 4)} \right] = \frac{-(a^2 - 1)n^4 - 4\sqrt{a^2 - 1}an^3 - (2a^2 + 1)n^2 + 8}{n^2(n^2 - 4)^2} < 0, \quad (\text{D5b})$$

$$\text{and } \frac{\partial(a - \sqrt{a^2 - 1})^{|n|}}{\partial n} = (a - \sqrt{a^2 - 1})^{|n|} \ln(a - \sqrt{a^2 - 1}) < 0 \quad (\text{D5c})$$

for any $|n| > 2$ and $a > 1$. Combining Eq. (D5), we conclude that $|h_3(a; L/R, n)|$ is monotonically decreasing with n in the region of interest, therefore its contributions to the eigenvalues and eigenfunctions problem is decreasing with n .

Now, let us compare the diagonal elements of $\tilde{\mathcal{H}}_{\text{free}}^{(2D)}$ with the nondiagonal ones. The ratio between the nondiagonal (15b) and diagonal (15a) elements is

$$\mathcal{R}^{(2D)}(a, n_2, n, m) \equiv \left| \frac{\langle \tilde{\mathcal{F}}_{n_2-n, m, k}^{(\Lambda)} | \hat{\mathcal{H}}_{\text{free}}^{(2D)} | \tilde{\mathcal{F}}_{n_2, m, k}^{(\Lambda)} \rangle}{\langle \tilde{\mathcal{F}}_{n_2, m, k}^{(\Lambda)} | \hat{\mathcal{H}}_{\text{free}}^{(2D)} | \tilde{\mathcal{F}}_{n_2, m, k}^{(\Lambda)} \rangle} \right| = \left| \frac{\frac{(|n|\sqrt{a^2-1}+a)(\sqrt{a^2-1}-a)^{|n|}}{(a^2-1)^{\frac{3}{2}}} (m^2 - \frac{1}{4})}{(n_2^2 - \frac{1}{4}) + \frac{a}{(a^2-1)^{\frac{3}{2}}} (m^2 - \frac{1}{4})} \right| \quad \text{for } n \neq 0. \quad (\text{D6a})$$

We denote

$$\mathcal{D}_1(a, n) \equiv (|n|\sqrt{a^2-1}+a)(\sqrt{a^2-1}-a)^{|n|}, \quad (\text{D6b})$$

and we have

$$\frac{\partial \mathcal{D}_1(a, n)}{\partial |n|} = (a - \sqrt{a^2-1})^{|n|} [(|n|\sqrt{a^2-1}+a) \ln(a - \sqrt{a^2-1}) + \sqrt{a^2-1}] \quad \text{and} \quad \frac{\partial \mathcal{D}_1(1, n)}{\partial |n|} = 0. \quad (\text{D6c})$$

However, since for $n \in \mathbb{Z} \setminus \{0\}$ and

$$\begin{aligned} & [(|n|\sqrt{a^2-1}+a) \ln(a - \sqrt{a^2-1}) + \sqrt{a^2-1}]_{a=1} = 0, \\ & \frac{\partial [(|n|\sqrt{a^2-1}+a) \ln(a - \sqrt{a^2-1}) + \sqrt{a^2-1}]}{\partial a} = \frac{(na + \sqrt{a^2-1}) \ln(a - \sqrt{a^2-1}) - n\sqrt{a^2-1}}{\sqrt{a^2-1}} \leq 0, \quad \text{for } \forall a \geq 1, \end{aligned} \quad (\text{D6d})$$

we conclude that the derivative $\partial \mathcal{D}_1(a, n)/\partial |n|$ is negative for any $n \in \mathbb{Z}$, $a > 1$, and $|n| \geq 1$, which implies that the nondiagonal terms (15b) decrease with $|n|$ for any a . Furthermore, since

$$\frac{\partial}{\partial a} \left[\frac{(|n|\sqrt{a^2-1}+a)}{(a^2-1)^{\frac{3}{2}}} \right] = -\frac{2a|n|\sqrt{a^2-1}+2a^2+1}{(a^2-1)^{\frac{5}{2}}} < 0 \quad \text{and} \quad \frac{\partial [(a - \sqrt{a^2-1})^{|n|}]}{\partial a} = -\frac{|n|(a - \sqrt{a^2-1})^{|n|}}{\sqrt{a^2-1}} < 0, \quad (\text{D6e})$$

than the nondiagonal terms (15b) decrease also with a and we have the asymptotic expression

$$\mathcal{R}^{(2D)}(a, n_2, n, m) \stackrel{a \gg 1}{\approx} \frac{1}{2^n a^{n+2}} \frac{n+1}{(n_2^2 - \frac{1}{4})} \left| m^2 - \frac{1}{4} \right|. \quad (\text{D7})$$

In conclusion, the ratio $\mathcal{R}^{(2D)}(a, n_2, n, m)$ (D6a) decreases with a , $|n|$, and $|n_2|$, as long as the diagonal term (15a) is positive. If $\mathcal{R}^{(2D)}(a, n_2, n, m) \ll 1$ for any $n \neq 0$, the nondiagonal terms may be neglected and the discussions of Secs. III D–III F apply to our problem.

To analyze the contribution of $\tilde{\mathcal{H}}_{A,2}^{(\xi)}$ to the eigenvalues and eigenfunctions problem of the Hamiltonian, let us assume that $\mathcal{R}^{(2D)}(a, n_2, n, m) \ll 1$ for any $n \neq 0$, so that the eigenfunc-

tions of $\tilde{\mathcal{H}}^{(2D)}$ are well approximated by $\tilde{\mathcal{F}}_{n_2, m, k}^{(\Lambda)}$ or $\tilde{\mathcal{F}}_{n_2, m, k}^{(\pm)}$, if $I/I_{\text{per}} = \eta/2$ (η integer). To estimate the contribution of the matrix elements of $\tilde{\mathcal{H}}_{A,2}^{(\xi)}$, we define

$$\mathcal{R}^{(\xi)}(a, n_2, n, m) \equiv \frac{I_{\text{per}}^2}{I^2} \left| \frac{\langle \tilde{\mathcal{F}}_{n_2 \pm n, m, k}^{(\Lambda)} | \tilde{\mathcal{H}}_{A,2}^{(\xi)} | \tilde{\mathcal{F}}_{n_2, m, k}^{(\Lambda)} \rangle}{\langle \tilde{\mathcal{F}}_{n_2, m, k}^{(\Lambda)} | \tilde{\mathcal{H}}_{\text{free}}^{(2D)} | \tilde{\mathcal{F}}_{n_2, m, k}^{(\Lambda)} \rangle} \right|, \quad (\text{D8a})$$

so that

$$\mathcal{R}^{(\xi)}(a, n_2, 0, m) = \left| \frac{h_0(a; L/R)}{n_2^2 - \frac{1}{4} + \frac{a}{(a^2-1)^{\frac{3}{2}}} (m^2 - \frac{1}{4})} \right|, \quad (\text{D8b})$$

$$\mathcal{R}^{(\xi)}(a, n_2, 1, m) = \left| \frac{h_1(a; L/R)}{n_2^2 - \frac{1}{4} + \frac{a}{(a^2-1)^{\frac{3}{2}}} (m^2 - \frac{1}{4})} \right|, \quad (\text{D8c})$$

$$\mathcal{R}^{(\xi)}(a, n_2, 2, m) = \left| \frac{h_2(a; L/R)}{n_2^2 - \frac{1}{4} + \frac{a}{(a^2-1)^{\frac{3}{2}}} (m^2 - \frac{1}{4})} \right|, \quad (\text{D8d})$$

$$\mathcal{R}^{(\xi)}(a, n_2, |n| > 2, m) = \left| \frac{h_3(a; L/R, n)}{n_2^2 - \frac{1}{4} + \frac{a}{(a^2-1)^{\frac{3}{2}}} (m^2 - \frac{1}{4})} \right|. \quad (\text{D8e})$$

For small currents, $(I/I_{\text{per}})^2 \ll [\mathcal{R}^{(\xi)}(a, n_2, n \neq 0, m)]^{-1}$ [for the values of a corresponding to Fig. 10, it is enough to check that $(I/I_{\text{per}})^2 \ll [\mathcal{R}^{(\xi)}(a, n_2, 2, m)]^{-1}$], the contribution

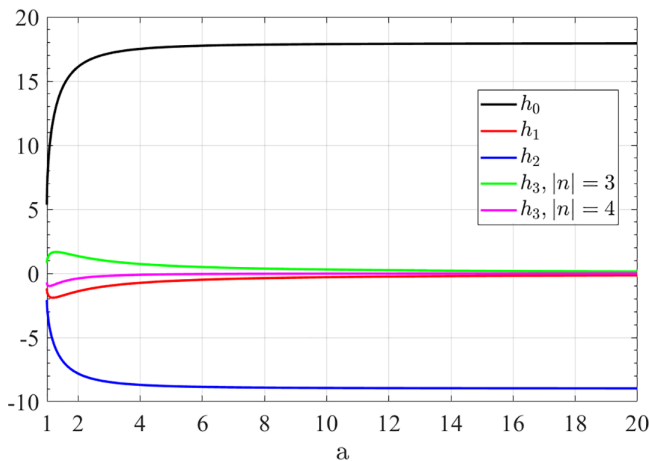


FIG. 10. The functions $h_0(a; L/R)/a^2$, $h_1(a; L/R)/a^2$, $h_2(a; L/R)/a^2$, and $h_3(a; L/R, n)/a^2$, for $n = 3, 4$ and $L/R = 10$.

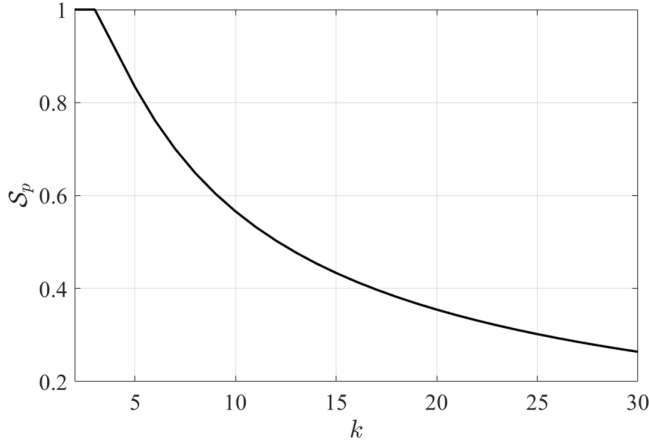


FIG. 11. The partial summation $\mathcal{S}_{\text{part}}(k)$ vs k . We observe a rapid decrease with k .

from the diagonal terms is dominant and the eigenfunctions are still well approximated by $\tilde{\mathcal{F}}_{n_2, m, k}^{(\Lambda)}$ or $\tilde{\mathcal{F}}_{n_2, m, k}^{(\pm)}$ [Eq. (35)]. In such a case, all the properties of the energy spectrum discussed in Secs. III D–III F are satisfied, except for the periodicity, since a term $(I/I_{\text{per}})^2 a^2 h_0(a; L/R)$ has to be added to all the energy eigenvalues. This quadratic dependence of the energy on the current is observed in the upper energy levels of Fig. 5, for example.

As I increases, when $(I/I_{\text{per}})^2$ becomes comparable to $[\mathcal{R}^{(\xi)}(a, n_2, n, m)]^{-1}$ for at least one value $n \neq 0$ [for the values of a corresponding to Fig. 10, we have the condition $(I/I_{\text{per}})^2 \approx [\mathcal{R}^{(\xi)}(a, n_2, 2, m)]^{-1}$, since $|\mathcal{R}^{(\xi)}(a, n_2, 2, m)| \geq |\mathcal{R}^{(\xi)}(a, n_2, n, m)|$ for any $n \neq 0$], the Hamiltonian matrix cannot be approximated anymore by its diagonal values and the eigenfunctions become significantly different from $\tilde{\mathcal{F}}_{n_2, m, k}^{(\Lambda)}$ or $\tilde{\mathcal{F}}_{n_2, m, k}^{(\pm)}$. This can be seen in Figs. 5 and 6, in the regions where the eigenvalues are not anymore quasidegenerate with the periodicity $I/I_{\text{per}} = 1/2$.

The situation is similar for the expectation values of $\tilde{T}_3$, presented in Fig. 7. Combining Eqs. (B13b), (20), and (29), we obtain the approximation (36) of the expectation values of the toroidal dipole at small currents [that is, when $(I/I_{\text{per}})^2 \ll [\mathcal{R}^{(\xi)}(a, n_2, n, m)]^{-1}$, for any $n \neq 0$]. The linear dependence of $\langle \tilde{T}_3^{(\theta)}(I) \rangle_{l, m, 1}$ on I and its abrupt changes around the current

values $I = (\eta/2)I_{\text{per}}$, where η is an integer, may be observed in Fig. 7, in regions where $(I/I_{\text{per}})^2 < [\mathcal{R}^{(\xi)}(a, n_2, n, m)]^{-1}$. Nevertheless, at transitions between different energy levels, say from the level l_1 to the level l_2 , the quantization observed in Eq. (29) remains valid, namely,

$$\langle \tilde{T}_3 \rangle_{l_2, m, 1} - \langle \tilde{T}_3 \rangle_{l_1, m, 1} = \frac{5}{2} [n_2(l_1) - n_2(l_2)] \quad (\text{D9})$$

is an integer multiple of the quanta 2.5, where $n_2(l_1), n_2(l_2)$ are given by Eq. (28). When $(I/I_{\text{per}})^2$ becomes comparable to $[\mathcal{R}^{(\xi)}(a, n_2, n, m)]^{-1}$ for some values of n , the current dependence of $\langle \tilde{T}_3^{(\theta)}(I) \rangle_{l, m, 1}$ changes qualitatively.

APPENDIX E: ANALYTICAL EXPRESSION FOR $I_n(a)$

To prove Eq. (B4), we first write

$$\begin{aligned} & \frac{1}{2} (I_{n+1} + I_{n-1}) + a I_n \\ &= \frac{1}{2\pi} \int_0^{2\pi} \frac{e^{in\theta} \frac{1}{2} (e^{i\theta} + e^{-i\theta}) + e^{in\theta} a}{a + \cos(\theta)} d\theta \\ &= \frac{1}{2\pi} \int_0^{2\pi} e^{in\theta} d\theta = \delta_n. \end{aligned} \quad (\text{E1})$$

If we assume that $I_n(a) \equiv C(a)\lambda^n(a)$, then, for $n > 0$ Eq. (E1) gives us the recurrence relation

$$\lambda^2 + 2a\lambda + 1 = 0, \quad (\text{E2})$$

with the general solutions

$$I_n(a) = C(a)(-a \pm \sqrt{a^2 - 1})^n.$$

Observing that

$$\begin{aligned} -a - \sqrt{a^2 - 1} &= \frac{1}{-a + \sqrt{a^2 - 1}}, \\ I_n &= I_n^* = I_{-n}, \quad \text{and} \quad I_0(a) > 0, \end{aligned} \quad (\text{E3})$$

we obtain the final solution

$$I_n(a) = \frac{(-a + \sqrt{a^2 - 1})^{|n|}}{\sqrt{a^2 - 1}}, \quad (\text{E4})$$

which is the first equation of Eq. (B4). The second equation of Eq. (B4) follows simply from the first one.

APPENDIX F: ASYMPTOTIC RELATIONS FOR $I_n^{(\ln^2)}(a)$ AND $\tilde{I}_n^{(\ln^2, \pm)}(a)$

Since $|\cos \theta/a| < 1$, we may write

$$\begin{aligned} I_n^{(\ln^2)}(a) &\equiv \frac{1}{2\pi} \int_0^{2\pi} e^{in\theta} \ln^2(a + \cos \theta) d\theta = \ln(a) \left[2 \ln \left(\frac{a + \sqrt{a^2 - 1}}{2} \right) - \ln(a) \right]_{n=0} - 2 \ln(a) \frac{(-a + \sqrt{a^2 - 1})^{|n|}}{|n|} \Big|_{n \neq 0} \\ &+ \sum_{k=2}^{\infty} \left\{ \left(\frac{-1}{2a} \right)^k \left[\sum_{l=1}^{k-1} \frac{1}{l(k-l)} \right] \left[\sum_{l=0}^k \binom{k}{l} \delta_{|n|, 2l-k} \right] \right\}. \end{aligned} \quad (\text{F1})$$

In Fig. 11, we plot the partial summation

$$\mathcal{S}_{\text{part}}(k) \stackrel{k \geq 2}{=} \sum_{l=1}^{k-1} \frac{1}{l(k-l)} = \frac{2}{k} \sum_{l=1}^{k-1} \frac{1}{l} \equiv \frac{2}{k} H_{k-1}, \quad \text{with} \quad \mathcal{S}_{\text{part}}(2) = \mathcal{S}_{\text{part}}(3) = 1 \quad \text{and} \quad \mathcal{S}_{\text{part}}(n > 3) < 1, \quad (\text{F2a})$$

where H_{k-1} is the harmonic number. Using this observation, we may write an asymptotic expression for $\mathcal{S}_{\text{part}}(k)$:

$$\mathcal{S}_{\text{part}}(k) \stackrel{k \gg 1}{\approx} \frac{2}{k} \left[\ln(k) + \gamma + \mathcal{O}\left(\frac{1}{k}\right) \right], \quad (\text{F2b})$$

where $\gamma \approx 0.57721$ is the Euler's constant.

Using Eq. (F2), we analyze the summation

$$\mathcal{S}(n) \equiv \sum_{k=2}^{\infty} \left\{ \left(\frac{-1}{2a} \right)^k \mathcal{S}_{\text{part}}(k) \left[\sum_{l=0}^k \binom{k}{l} \delta_{|n|, 2l-k} \right] \right\} \equiv \sum_{k=2}^{\infty} \mathcal{S}_1(n, k), \quad (\text{F3a})$$

from Eq. (F1) and write its expressions for even and odd n :

$$\mathcal{S}(n) \equiv \sum_{t=\max(s, 1)}^{\infty} \left\{ \left(\frac{1}{2a} \right)^{2t} \frac{(2t)!}{(t+s)!(t-s)!} \mathcal{S}_{\text{part}}(2t) \right\}, \quad \text{for } |n| \equiv 2s, \quad (\text{F3b})$$

$$\mathcal{S}(n) \equiv - \sum_{t=\max(s, 1)}^{\infty} \left\{ \left(\frac{1}{2a} \right)^{2t+1} \frac{(2t+1)!}{(s+t+1)!(t-s)!} \mathcal{S}_{\text{part}}(2t+1) \right\}, \quad \text{for } |n| \equiv 2s+1, \quad (\text{F3c})$$

where $s \geq 0$ is an integer. The convergence of the summations in Eqs. (F3) can be readily demonstrated by analyzing the asymptotic behavior of $\mathcal{S}_1(n, k)$. For $k, k-n \gg 1$, we may use the Stirling approximation for the factorials, treating n as a continuous variable in Eq. (F3a), whereas for $n/k \ll 1$ we may use the Taylor expansion. Then, the logarithm of the absolute value of a term of the summation $\mathcal{S}(n)$ may be approximated as

$$\ln [|\mathcal{S}_1(n, k)|] = \ln \left\{ \left(\frac{1}{2a} \right)^k \mathcal{S}_{\text{part}}(k) \frac{k!}{\left(\frac{k+n}{2}\right)! \left(\frac{k-n}{2}\right)!} \right\} \approx \ln[\mathcal{S}_{\text{part}}(k)] - k \ln(a) - \frac{n^2}{k}, \quad (\text{F4a})$$

which leads to

$$|\mathcal{S}_1(n, k)| \approx \mathcal{S}_{\text{part}}(k) e^{-n^2/k} a^{-k}. \quad (\text{F4b})$$

Therefore, the series (F3) decrease more rapidly than a geometric progression with common ratio $a^{-1} < 1$, leading to the conclusion that these series are absolutely convergent. On the other hand, from any of Eqs. (F3) it follows that $k \geq |n|$, therefore, for any n the lowest order term is

$$\mathcal{S}_1(n, |n|) = \left(\frac{-1}{2a} \right)^{|n|} \mathcal{S}_{\text{part}}(|n|). \quad (\text{F4c})$$

The other nonzero term from Eq. (F1) has the asymptotic expansion:

$$-2 \ln(a) \frac{(-a + \sqrt{a^2 - 1})^{|n|}}{|n|} \Big|_{n \neq 0} \stackrel{a \gg 1}{\approx} - \left(\frac{-1}{2a} \right)^{|n|} 2 \ln(a) \left(\frac{1}{|n|} + \frac{1}{4a^2} + \mathcal{O}\left(\frac{1}{na^4}\right) \right). \quad (\text{F4d})$$

Therefore, from Eqs. (F4c) and (F4d), we see that the dominant term in the expansion of $I_n^{(\ln^2)}(a)$ with respect to a is

$$\left(\frac{-1}{2a} \right)^{|n|} \left[\mathcal{S}_{\text{part}}(|n|) - \frac{2 \ln(a)}{|n|} \right], \quad \text{for any } |n| \geq 2, \quad (\text{F5})$$

which explains the rapid decrease of $|I_n^{(\ln^2)}(a)|$ with increasing values of both n and a .

The results above may be readily applied to obtain the asymptotic behavior of $\tilde{I}_n^{(\ln^2)}(a)$. For $|n| \leq 4$, the dominant terms are given in Eq. (B10c), whereas for $|n| \geq 4$, we use the identity $\tilde{I}_n^{(\ln^2, \pm)}(a) \equiv I_n^{(\ln^2)}(a) \pm [I_n^{(\ln^2)}(a) + I_n^{(\ln^2)}(a)]/2$ and Eq. (F5):

$$\tilde{I}_n^{(\ln^2, \pm)}(a) \stackrel{|n| \geq 4}{\approx} \pm \frac{1}{2} \left(\frac{-1}{2a} \right)^{|n|-2} \left[\mathcal{S}_{\text{part}}(|n|-2) - \frac{2 \ln(a)}{|n|-2} \right], \quad (\text{F6})$$

where the result for $|n| = 4$ is identical to the one in Eq. (B10c).

APPENDIX G: MATRIX ELEMENTS IN THE SYMMETRIC AND ANTISYMMETRIC BASIS

For $I/I_{\text{per}} = \eta/2$ (with η an integer), in the symmetric/antisymmetric basis defined in Eq. (31), the matrix elements of the free Hamiltonian are calculated by combining the results from Eq. (15). For the off-diagonal coupling between parity sectors, we find

$$\langle \tilde{\mathcal{F}}_{n_1^{(D)}, m_1, k_1}^{(+)} | \tilde{\mathcal{H}}_{\text{free}}^{(2D)} | \tilde{\mathcal{F}}_{n_2^{(D)}, m_2, k_2}^{(-)} \rangle = 0, \quad (\text{G1})$$

confirming the block-diagonal structure of the Hamiltonian. The nonzero diagonal elements within each parity block are

$$\langle \mathcal{F}_{n_2^{(j)},m,k}^{(\pm)} | \tilde{\mathcal{H}}_{\text{free}}^{(2D)} | \mathcal{F}_{n_2^{(j)},m,k}^{(\pm)} \rangle = a^2 \left[(n_2^{(j)})^2 - \frac{1}{4} + \frac{a \pm (2n_2^{(j)} \sqrt{a^2 - 1} + a)(\sqrt{a^2 - 1} - a)^{2n_2^{(j)}}}{(a^2 - 1)^{\frac{3}{2}}} \left(m^2 - \frac{1}{4} \right) \right]. \quad (\text{G2})$$

The energy splitting in Eq. (34) is derived directly from the difference between the (+) and (−) diagonal elements in Eq. (G2).

For the toroidal dipole operator $\tilde{T}_3$, we exploit the symmetry relation of the original matrix elements [Eq. (B14)]:

$$\langle \mathcal{F}_{n_1^{(j)},m,k}^{(\Lambda)} | \tilde{T}_{3,0}^{(\xi)} | \mathcal{F}_{n_2^{(j)},m,k}^{(\Lambda)} \rangle = -\langle \mathcal{F}_{n_1^{(j)},m,k}^{(\Lambda)} | \tilde{T}_{3,0}^{(\xi)} | \mathcal{F}_{-n_2^{(j)},m,k}^{(\Lambda)} \rangle. \quad (\text{G3})$$

Applying this to the symmetric basis vectors, we obtain

$$\langle \tilde{\mathcal{F}}_{n_1^{(j)},m,k}^{(+)} | \tilde{T}_3(I=0) | \tilde{\mathcal{F}}_{n_2^{(j)},m,k}^{(+)} \rangle = \langle \tilde{\mathcal{F}}_{n_1^{(j)},m,k}^{(-)} | \tilde{T}_3(I=0) | \tilde{\mathcal{F}}_{n_2^{(j)},m,k}^{(-)} \rangle = 0. \quad (\text{G4})$$

This proves that the expectation value of the toroidal dipole is strictly zero for any state with definite parity.

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