Exploiting Oriented Field Projectors to Open Topological Gaps in Plasmonic Nanoparticle Arrays

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ABSTRACT: In the last years there have been multiple proposals in nanophotonics to mimic topological condensed matter systems. However, nanoparticles have degrees of freedom that atoms lack of, like dimensions or shape, which can be exploited to explore topology beyond electronics. Elongated nanoparticles can act like projectors of the electric field in the direction of the major axis. Then, by orienting them in an array the coupling between them can be tuned, allowing to open a gap in an otherwise gapless system. As a proof of the potential of the use of orientation of nanoparticles for topology, we study 1D chains of prolate spheroidal silver nanoparticles. We show that in these arrays spatial modulation of the polarization allows to open gaps, engineer hidden crystalline symmetries and to switch on/off or left/right edge states depending on the polarization of the incident electric field. This opens a path toward exploiting features of nanoparticles for topology to go beyond analogues of condensed matter systems.

KEYWORDS: topological photonics, plasmonics, nanoparticle arrays, edge states, surface plasmons

INTRODUCTION

The exciting discovery of the topological phase of matter systems has inspired many new fields in physics, particularly in photonics. In fact, in recent years, we have witnessed an exponential growth of interests in that direction. Mimicking the phenomenology of topological insulators has been the driving force until now. However, it is becoming clear that a further step needs to be taken, that is, to push forward new topological photonic phenomenology that does not have a material counterpart.

Topological insulators are possible thanks to the Fermionic nature of electrons, but photons cannot take advantage of such symmetry. Initial solutions have been proposed based on gyromagnetic photonic crystals, bianisotropic materials, and coupled waveguides and resonators.

All the previous systems use some kind of time-reversal property not present in simple photonics systems without magnetic response. In addition, there is always a strong interest in achieving very small and faster devices for nanotechnological applications. Typical examples are microprocessors, but light interacts weakly with the material at the nanoscale. Moreover, one would like to have such photonic properties in the visible, where most of the molecular electronic transitions happens, making such zone relevant in light-matter interaction. With these goals and restriction in mind, metal nanoparticles using plasmonic resonances are probably the best candidates. This has made it possible for many researchers to look at what we can call topological nanoparticle photonics.

Plasmonic nanoparticles provide an excellent platform for light-matter interaction, but being not simple to break time-reversal symmetry in the visible range, a typical approach is using crystal symmetries. Such an approach has also been explored for radiative heat transfer with interesting results.

In addition, particular care needs to be taken due to the long-range nature of these interactions and the radiative corrections, which can spoil the topological protection of the system. Here, instead of focusing on such loss of protection, we explore degrees of freedom of the nanoparticles which could be exploited for topology beyond condensed matter systems.

This paper is organized as follows. In the first section we introduce the simplest topological system, a dimer chain known as SSH model, and its extensions for larger unit cells. In the second section we study and compare different plasmonic counterparts of these chains. In last section we discuss the
SSH MODEL AND TOPOLOGICAL PHASES

The Su-Schrieffer-Heeger (SSH) model is the simplest system with topological protection. It was first proposed in ref 20 to describe the physics of the polyyacetylene chain, which alternates double and simple (or strong and weak) bonds between adjacent carbon atoms. In Figure 1a we show a scheme of this model, which consists of a one-dimensional diatomic chain with two staggered hopping amplitudes between nearest neighbors, namely, \( v \) and \( w \). Its tight-binding Hamiltonian is

\[
\mathcal{H}(q) = \begin{pmatrix} 0 & v + we^{-iqd} \\ v + we^{iqd} & 0 \end{pmatrix}
\]

and satisfies the Schrödinger equation:

\[
\mathcal{H}(q) |u_n(q)\rangle = E_n(q) |u_n(q)\rangle
\]

This system has two different distinct topological phases: it is trivial when the bond between particles in adjacent unit cells is weaker than the one between particles within a unit cell (\( |w| < |v| \)) and topological when it is stronger (\( |w| > |v| \)). When we choose the periodic chain commensurately with the topological unit cell, it hosts strongly localized zero-energy states at both ends. These edge states are robust to disorder and perturbations that respect its symmetries: sublattice symmetry (also known as chirality) and mirror/inversion symmetries. Sublattice symmetry stems from the existence of two sublattices (\( A \) and \( B \)) with bonds between sublattices but not within a sublattice. This implies the Hamiltonian is antiblock-diagonal, i.e.:

\[
\mathcal{H}(q) = \begin{pmatrix} 0 & h(q) \\ h^*(q) & 0 \end{pmatrix}
\]

Chirality makes the spectrum symmetric around zero energy and fixes the energy of the edge states at zero, isolating them from the bulk states. It also makes each edge state be localized in just one of the sublattices.

\[
\Gamma \mathcal{H}(q) \Gamma = -\mathcal{H}(q) \quad \Gamma = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]

(4)

The SSH model is mirror-symmetric because the system remains invariant under spatial inversion in the x-axis, i.e., under the operation of \( \Pi \):

\[
\Pi \mathcal{H}(q) \Pi = \mathcal{H}(\bar{q}) = \mathcal{H}(q)
\]

(5)

The SSH chain is also inversion-symmetric, as it remains invariant under the subsequent spatial inversion in all axes. Mirror or inversion symmetries lead to the double degeneracy of the edge states, even when the sublattice symmetry is broken.

As long as chirality and mirror symmetries are respected, the Zak phase \( \gamma \), a bulk property, is a topological invariant and predicts the existence of edge states in the terminated system. This is known as bulk-boundary correspondence. The Zak phase for each band and for the gap is

\[
\gamma_n = \int_{BZ} \langle u_n(q) | \frac{\partial}{\partial q} | u_n(q) \rangle dq
\]

\[
\gamma = \sum_{\text{below gap}} \gamma_n
\]

(6)

In electronic systems, when the system is neutral, only half of the bands are below the Fermi level, so in the SSH model only the lower band contributes to the Zak phase.

In the following subsection we introduce some extensions of the SSH model.

Extended Unit Cell SSH Models. Due to the simplicity of the system, several generalizations of the SSH model have been made, for example, by adding hoppings between further neighbors or by extending to two dimensions in a square array. This model can also be generalized to one-dimensional chains with larger linear unit cells or rhombus unit cells. These systems are topologically more complex than the SSH model, featuring several gaps and nonzero edge states. They can also exhibit other kinds of topological protection like square-root topology.

First, as we show in Figure 1b, we consider a linear chain with three alternating hopping amplitudes \( u, v, \) and \( w \). This lattice has three different sublattices \( A, B, \) and \( C \). The topology of this system has been discussed in refs 28, 31, and 32.

\[
\mathcal{H}(q) = \begin{pmatrix} 0 & u & we^{-iqd} \\ u & 0 & v \\ we^{iqd} & v & 0 \end{pmatrix}
\]

(7)

A three-way generalization of the sublattice symmetry can be made for this chain:

\[
\Gamma_3^{-1} \mathcal{H}(q) \Gamma_3 + \Gamma_3^{-2} \mathcal{H}(q) \Gamma_3^2 = -\mathcal{H}(q)
\]

(8)

This symmetry is the same that features the breathing Kagome lattice. However, due to the absence of the \( C_3 \) rotational symmetry also present in the Kagome lattice, in this 1D system there are not three degenerate zero-states but four nonzero edge states. Additionally, the edge states are not localized in...
just one of the sublattices but the two closer to the edge. When the chain is mirror symmetric, i.e., $|u| = |v|$, the edge states come in two degenerate pairs at energies $-E$ and $E$ when $|w| > |u|$. Each gap has a distinct Zak phase that is quantized by mirror symmetry. Due to the three-way chirality, they are not independent, but the same.

Similarly, we can consider a chain with a 4-particle unit cell, shown in Figure 1c, with hoppings $t$, $u$, $v$, and $w$. The tight-binding Hamiltonian (in the base $A$, $C$, $B$, $D$) is

$$H(q) = \begin{pmatrix} 0 & 0 & t & we^{-iqd} \\ 0 & 0 & u & v \\ t & u & 0 & 0 \\ we^{-iqd} & v & 0 & 0 \end{pmatrix}$$

(9)

Due to the even number of particles in the unit cell, this chain recovers the sublattice symmetry from the SSH model. The transition for the central gap occurs when $|tv| = |uw|$. When $|tv| > |uw|$ the system is in the trivial phase, whereas for $|tv| < |uw|$ the system has symmetry-protected zero-energy states that localize exclusively in even or odd sublattices.

However, the system also features nonzero energy states in the lower/upper gaps. These states inherit properties from the four-way generalized chirality, which is given by

$$\Gamma_4^{-1}H(q)\Gamma_4 + \Gamma_4^{-2}H(q)\Gamma_4^2 + \Gamma_4^{-3}H(q)\Gamma_4^3 = -H(q),$$

$$\Gamma_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -i \end{pmatrix}, \quad \Gamma_4^* = I$$

(10)

This symmetry makes the nonzero edge states be localized in three out of the four sublattices. However, this symmetry does not close lower/upper gaps or quantize their Zak phases, but spatial symmetries do. The system is mirror/inversion symmetric when $|t| = |v|$. Mirror symmetric nonzero energy edge states appear for $|w| > |u|$. Mirror symmetric nonzero energy edge states appear for $|w| > |u|$.

## TOPOLOGICAL PLASMONIC CHAINS

### Coupled-Dipole Equations

Now we focus in arrays of plasmonic nanoparticles. Previously, optical response of metallic nanoparticles has been used to mimic topological condensed matter systems, as in zigzag chains,\textsuperscript{35,36} diatomic chains of nanospheres,\textsuperscript{37} or breathing Kagome\textsuperscript{38} and breathing honeycomb plasmonic metasurfaces.\textsuperscript{39,40} However, in these systems it has been shown that long-range interactions between nanoparticles must be considered, which have a striking effect on the topology of the system.\textsuperscript{18,19}

Electric fields produce localized surface plasmon resonances (LSPR) in metallic nanoparticles. A small single nanoparticle with $a \ll \lambda$ (where $a$ is the particle radius and $\lambda$ is the...
wavelength of incoming light) scatters an incident electric field $E_{\text{inc}}$ approximately like a dipole $p$:

$$p = \varepsilon_0 \alpha(\omega) E_{\text{inc}}$$

(11)

where $\varepsilon_0$ is the permittivity of the background medium and $\alpha(\omega)$ is the polarizability tensor.

We choose particles such that $a > 3 - 4$ nm to avoid quantum effects. However, to take into account these quantum effects in a simple way, a solution is to follow the prescription of Kreibig that showed how the finite size affects the electron free path.41

The dipolar approximation still holds for an array of nanoparticles, if they are separated a distance of at least $3a$. Then, each dipole in the array is determined by both the incident electric field and the scattered electric field by the rest of the dipoles:

$$p_n = \alpha_n(\omega) \left[ E_{\text{inc}} + \frac{k^2}{\varepsilon_0} \sum_{m \neq n} G(r_{nm}, r_{nm}, \omega) p_m \right]$$

(12)

where $n, m$ are sites in the array, $p_{n,m}$ are the dipoles in positions $r_{nm}$ and $G(r_{nm}, r_{nm}, \omega)$ is the Green’s dyadic function, which in the quasi-static regime $kR \gg 1$ is given by

$$G(r_{nm}, r_{nm}, \omega) = \frac{1}{4\pi k^2 R^3} \left[-I + \frac{3}{2} \frac{R \otimes R}{R^3} \right]$$

(13)

where $R = r_n - r_m$, $R = |R|$, and $k = \sqrt{\varepsilon_0 \omega/c}$ is the wavevector.

In the next subsections we will consider examples of topological arrays of nanoparticles.

**Chain of Nanospheres.** First, we consider a single spherical metallic nanoparticle. A nanosphere has a spherical symmetry, so its tensor polarizability behaves like a scalar, $\alpha(\omega)$, which in the quasi-static limit $a \ll \lambda$ is

$$\alpha(\omega) = 4\pi \varepsilon_0 \varepsilon_1(\omega) - \varepsilon_\infty + 2\alpha_\infty$$

(14)

In Figure 2a we see the optical response of a single silver nanosphere of radius $a = 12.5$ nm to a linear-polarized electric field (blue curve), that shows a resonance for $\hbar \omega_{sp} \sim 2.75$ eV.

Now we consider a plasmonic analogue of the SSH model, i.e., a chain of nanospheres with two alternate distances: the intracell distance $\beta_2$ and the intercell distance $(2 - \beta)^{-d/2}$, $d$ being the size of the unit cell (see scheme on Figure 2b). For any array of nanospheres and in the absence of incident electric field, we can rewrite eq 12 as

$$\frac{1}{\alpha(\omega)} p_n = \frac{k^2}{\varepsilon_0} \sum_{m \neq n} G(r_{nm}, r_{nm}, \omega) p_m$$

(15)

After Bloch, coupled-dipole equations can be compacted in a matrix equation:

$$G(q)P = \frac{1}{\alpha(\omega)} P$$

(16)

where $P = (P_{1s}, P_{2s}, P_{1p}, P_{2p}, P_{1f}, P_{2f}, P_{1z}, P_{2z})$.18 As we see, this is equivalent to the Schrödinger equation in eq 2, where the dipole vector, the inverse of the polarizability, and the Green’s matrix $G(q)$ take the roles of, respectively, eigenvectors, eigenvalues, and the Bloch Hamiltonian $H(q)$. Explicitly, $G(q)$ terms are

$$G_{\mu\nu} = \delta_{\mu\nu} \frac{2m}{\varepsilon_\infty R^3} \left[ \frac{1}{\beta^3} + \frac{1}{(2 - \beta)^3} e^{-qR} \right]$$

(17)

where $\mu, \nu = x, y, z$ are the polarizations of each pair of dipoles, and $m_1 = m_2 = 2$ for the longitudinal polarization and $m_1 = m_2 = -1$ for the transversal polarizations. This is, the plasmonic dimer chain of nanospheres is equivalent to three independent copies of the SSH (eq 1), one per polarization, with $v = \frac{2m}{\varepsilon_\infty R^3}$ and $\omega = \frac{2m}{\varepsilon_\infty R^3} \beta$. The dispersion bands $\omega(q)$ can be calculated from eq 16, searching for the solutions of

$$\lambda_n - \frac{1}{\alpha(\omega)} = 0$$

(18)

$\lambda_n$ being the $n$th eigenvalue of $G(q)$. The zero-energy modes typical of the finite SSH model translate in this system to six (two per polarization) resonant modes localized at the edges of the chain at the surface plasmon frequency of a single nanosphere $\omega_{sp}$.42

Apart from the plasmonic diatonic 1D chain, the zigzag chain,35 which alternates angles between the nanoparticles, has also been proposed to mimic the topology of the SSH model. This system exploits the polarization asymmetry between longitudinal and transversal modes and allows to select edge modes by changing the polarization of the incoming electric field. In the next subsection we will get advantage of this same anisotropy not in the geometry of the array but in the shape of the nanoparticles, adding a new degree of freedom to the system.

**Chain of Nanospheroids.** When the nanoparticles are not spherical, $\alpha(\omega)$ tensors are not proportional to the identity matrix anymore, so they affect the polarization of the dipoles. This asymmetry has no analogy in tight binding models and can be exploited to explore new topological systems. For example, if we replace the nanospheres in the previous chain by parallel nanorods, we can filter modes by in-plane or out-of-plane polarizations. However, by orienting the nanoparticles in different directions, we can force modes beyond the plasmonic nanosphere chain.

Previously, gradual change of orientation in arrays of anisotropic nanoparticles or nanoholes has been exploited in Pancharatnam-Berry metasurfaces (also known as geometric phase metasurfaces) for example to enable polarization-dependent control of light45 or to create vortex beams.3170

Here we use orientation of elongated nanoparticles not to build a geometric phase in polarization, but to tune the interactions between nanoparticles in order to open a topological gap. However, the spatial modulation of polarization in our system plays a role in the control of edge states, allowing to switch them off by changing the polarization of the incident electric field, as we will see in last section.

The strategy pursued in this paper to open a topological gap is similar to in ref 44, where it is opened by orientation in the transversal plane of bianisotropic particles in an equidistant array. However, our study is more general and in the visible range.

Let us now assume our elongated nanoparticles are prolate spheroidal nanoparticles with axis half-lengths $a > b = c$ with.
the major axis pointing in the z direction. The results will be qualitatively equivalent for any other elongated shape, so we’re not losing generality by making this choice. In this case the polarizability tensor is

\[
\mathbf{\alpha}(\omega) = \begin{pmatrix}
\alpha_1(\omega) & 0 & 0 \\
0 & \alpha_2(\omega) & 0 \\
0 & 0 & \alpha_3(\omega)
\end{pmatrix}
\]

(19)

where the quasistatic polarizabilities \( \alpha_l \) with \( l \in [a, b, c] \) are \( \alpha_l(\omega) = V \frac{e_l(\omega) - e_b}{e_b + L_l(e(\omega) - e_b)} \)

(20)

where \( V \) being the volume of the spheroid, \( V = \frac{4}{3} \pi a c^2 \), and \( L_l \) are geometric factors (see Supporting Information).

In Figure 2a we can see the extinction cross section (see Supporting Information for details) of a single silver nanospheroid with major axis \( a = 12.5 \text{ nm} \) and minor axis \( b = c = 0.4a = 5 \text{ nm} \). Red curve represents the response to a field polarized parallel to the major axis, while for the green curve the field is polarized normal to the major axis. As we see, the resonance wavelengths are separate enough (\( h\omega_{\text{res}} \sim 2.96 \text{ eV} \), whereas \( h\omega_{\text{res}} \sim 2.0 \text{ eV} \)), that in the proximity of the major axis resonance, \( \alpha_1(\omega \approx \omega_{\text{res}}) \approx 0 \), so we can approximate the tensor polarizability to

\[
\mathbf{\alpha}(\omega \approx \omega_{\text{res}}) \approx \begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & \alpha_3(\omega)
\end{pmatrix}
\]

(21)

This means the polarizability tensor acts like a projection operator, projecting the dipole in the direction of the major axis.

Now we consider an array of nanospheroids, with the major axis oriented in the directions \( \mathbf{u}_n = (\cos \phi_n, \sin \phi_n, 0)^T \), where \( \phi_n \) is the angle of the particle \( n \) with respect to the x axis. We assume all the particles are oriented in the plane xy for the sake of simplicity. As y and z axes are indistinguishable, all results will be the same for the xz plane. The equations for the general case, with nanoparticles oriented in any direction, are in the Supporting Information.

Due to the projection of the polarizability in the directions of the major axes of the particles, the vectorial coupled-dipole equations in an array of nanospheroids can be reduced to scalar equations:

\[
\frac{1}{\alpha_3(\omega)} P_n = \frac{k^2}{c_0} \sum_{m \neq n} G_{u_n, u_m} P_m
\]

(22)

where \( G_{u_n, u_m} = \left( \mathbf{G}(r_{nm}, \mathbf{u}_m, \omega), \mathbf{u}_n \right) \cdot \mathbf{u}_m \) is the projection of the polarizability tensor in the directions \( \mathbf{u}_m, \mathbf{u}_n \).

The coupled-dipole equations can again be rewritten in a matrix form:

\[
\mathbf{G}(k) P = \frac{1}{\alpha_3(\omega)} P
\]

(23)

where in this case \( \mathbf{G}(k) \) is a \( N \times N \) matrix with elements given by \( G_{u_n, u_m} \) and \( P = (|p_1|, ..., |p_N|) \) is a vector containing the module of the dipoles.

First, let us consider a 1D chain of equidistant nanoparticles, separated by a distance \( R \). We can see an scheme of this chain in Figure 2c. As all the particles are in the x axis, the Green dyadic’s function reduces to

\[
\mathbf{G}(r_{nm}, \mathbf{u}_n) = \begin{pmatrix}
2 & 0 & 0 \\
0 & -1 & 0 \\
0 & 0 & -1
\end{pmatrix}
\]

(24)

and its projection onto the \( \mathbf{u}_n \) and \( \mathbf{u}_j \) axes is

\[
G_{u_n, u_m} = \frac{2 \cos \phi_m \cos \phi_n - \sin \phi_m \sin \phi_n}{4\pi k^2 R^4}
\]

(25)

This means that we can tune the coupling between nanoparticles by rotating them. In Figure 2d we plot the interaction \( G_{u_n, u_m} \) multiplied by \( 4\pi k^2 R^4 \), depending on the orientation angles \( \phi_m \) and \( \phi_n \). This interaction ranges from 2 (parallel dipoles in the longitudinal direction) to \(-2\) (antiparallel and in the longitudinal direction), passing by \(-1\) (parallel dipoles in the transversal polarization). For any pair of angles in the zero contour line, the interaction is suppressed. For example, orthogonal nanospheroids oriented in the \( x \) and \( y \) directions do not interact between them, as we see for \( \phi_1 = 0, \phi_2 = \frac{\pi}{2} \) or vice versa in the colormap.

This zero interaction was impossible to achieve in the nanosphere chain and it could only be approximated by separating the particles a long distance (see eq 17). This could be interesting for switching off some even neighbor interactions that can break sublattice symmetry, but here we will restrict to the first-neighbor approximation. This approximation is accurate only in the quasi-static regime, that is, when the nanoparticles and the distances between them are small, so \( kR \ll 1 \).

In the next subsections we will consider linear arrays of nanospheroids. With nanospheres, a linear chain where the nanoparticles were equidistant would be gapless and equivalent to the \( v = w \) case in the SSH model. However, by substituting the nanospheres with nanospheroids and adding the orientation as a degree of freedom, a gap can be opened.

**Two Particles/Unit Cell.** First we consider the simplest system that may have a topological gap. This is a linear array with two particles/unit cell and with a distance between adjacent particles \( R = \frac{d}{2} \), with \( d \) being the size of the unit cell. For nanospheroids, the Green matrix of the system would be

\[
\mathbf{G}(q) = G_{u_n, u_m} \begin{pmatrix}
0 & 1 + e^{-iqd} \\
1 + e^{iqd} & 0
\end{pmatrix}
\]

(26)

This system is equivalent to the SSH model with \( v = w = G_{u_n, u_m} \) due to the reciprocity \( G_{u_n, u_m} = G_{u_m, u_n} \). This means that by rotating the spheroidal nanoparticles in a two-particle unit cell, we can change the amplitude of the bands, but not open a gap.

**Three Particles/Unit Cell.** However, if we enlarge the unit cell, we can open a gap in an array of equidistant particles. Let us consider a three-particle unit cell with \( R = \frac{d}{3} \). Then the Green dyadic’s matrix is
Figure 3. Plasmonic analogue of the mirror-symmetric SSH3 model: periodic chain of three prolate silver nanospheroids per unit cell, with long spheroidal axes forming angles with the chain direction $\varphi_k = \varphi_0 - \frac{\pi}{2} = \varphi_e$. The dimensions of the nanoparticles are $a = 12.5 \text{ nm}$ and $b = c = 0.4a = 5 \text{ nm}$ and the interparticle distance is $R = \frac{d}{3} = 5a$. (a) Unit cells for $\varphi = -\frac{\pi}{4}$, $\varphi = 0$, and $\varphi = \frac{\pi}{4}$. For any $\varphi$, the unit cell is inversion symmetric. (b) Equivalent tight binding unit cells. Solid and dashed black lines strong and weak hoppings. (c) Plasmonic bands of the periodic system. Solid lines represent the bands for $\varphi = 0$, dashed ones represent the bands for $\varphi = -\frac{\pi}{4}$ and dotted lines are $\varphi = -\varphi_e, \varphi_0$, with $\varphi_e \sim 0.16\pi$, where the lower and upper gaps close and topological transitions occur. (d) Plasmonic spectrum of a finite chain of 99 nanoparticles (33 unit cells). Bulk states are represented by blue lines, while green curves represent the two pairs of three-way-chiral edge states, that appear between $-\varphi_l$ and $\varphi_l$. Green dot marks the values corresponding to the edge state plotted in panel (f). (e) $\gamma$ Zak phase of lower/upper gaps, which matches with the existence of edge states in panel (d). (f) Lower gap edge state for $\varphi = -\frac{\pi}{4}$. The gradient represents the module of the dipoles in absence of incident field. Due to the three-way chirality the edge state is localized at the two sublattices closer to each edge.

\[
G(q) = \begin{pmatrix}
0 & G_{u_a u_a} e^{-iqld} & G_{u_a u_c} e^{-iqld} \\
G_{u_a u_a} & 0 & G_{u_b u_c} e^{iqld} \\
G_{u_a u_c} e^{iqld} & G_{u_b u_c} & 0
\end{pmatrix}
\] (27)

which is equivalent to the Bloch Hamiltonian of the SSH3 model (eq 7). The condition for the unit cell to be mirror-symmetric is $\varphi_A = -\varphi_C$ and $\varphi_B = 0, \frac{\pi}{2}$. The condition for the unit cell to be inversion-symmetric is, however, less restrictive. As a single nanospheroid is inversion-symmetric, the only condition is that particles $A$ and $C$ are inversion-symmetric with respect to each other, that is $\varphi_A = \varphi_C$.

The condition for $G(q)$ to be equivalent to the mirror-symmetric SSH3 is $|G_{u_a u_a}| = |G_{u_a u_c}|$. This is satisfied by any two pairs of angles $\varphi_B$, $\varphi_B$ and $\varphi_B$, $\varphi_C$ that lay on the same or opposite contour line in Figure 2d. Explicitly, this occurs for $\varphi_B = \arctan \left( \frac{2\cos \varphi_A \pm \cos \varphi_A}{\sin \varphi_A \pm \sin \varphi_A} \right)$. This includes mirror symmetric and inversion symmetric previous conditions, however, it goes beyond them. For example, if we fix $\varphi_A = 0, \varphi_C = \frac{\pi}{2}$, then the Green dyadic is accidentally mirror symmetric for $\varphi_B \sim 0.43\pi$ and $\varphi_B \sim 0.78\pi$.

This accidental symmetry stems from the fact that we are ignoring the orientation of the nanoparticles in the equations, so it is a symmetry of the strength of the interaction between particles. Due to the anisotropy between longitudinal and transversal modes, these symmetries happen for apparently random values of the orientations. However, this accidental symmetry is enough to quantize the Zak phase, as in the true mirror symmetric and inversion symmetric cases.

In Figure 3 we show the topological transition in this plasmonic analogue of the mirror-symmetric SSH3 model with $a = 12.5 \text{ nm}$, $d = 15a$, and $R = \frac{d}{3} = 5a$. By orienting the nanoparticles at $\varphi = \varphi_0, \varphi_C, \varphi_e = \varphi_0 - \frac{\pi}{2}$, upper and lower gaps close when $|G_{u_a u_a}| = |G_{u_a u_c}| = |G_{u_b u_c}|$, that is, for $\varphi = \pm \varphi_l \sim \pm 0.16\pi$. For $|\varphi_l| > \varphi_l$ and $|G_{u_a u_a}| < |G_{u_a u_c}|$, the system is in the trivial phase, while for $|\varphi_l| < \varphi_l$ and $|G_{u_a u_a}| > |G_{u_a u_c}|$ there are edge states in the upper/lower gaps, which frequency is not fixed at $\omega_{pla}$ and depends on the parameters, because they are not protected by sublattice symmetry. This makes them more tunable but less robust than the edge states in the SSH, as they can be more easily pushed into the continuum and hybridize with bulk states. However, we expect this kind of edge states to still be robust to weak off-diagonal disorder, as the edge states from rhombus chains.29

The appearance of these edge states matches the steps in the Zak phase, shown in panel (e). We also show one of the edge states of the lower gap for $\varphi = -\frac{\pi}{30}$ in Figure 3f, which as we see inherits the symmetry of the three-way chirality, localizing in the two sublattices closer to the edge.

Interestingly, the asymmetry of transversal and longitudinal Green dyadic's functions can be exploited not just to open a gap but also to engineer accidental spatial symmetries or to suppress interaction between particles. This system is therefore more flexible than the linear and zigzag chains of nanospheres, allowing to play with symmetries, which yield a response of the system is in the trivial phase, while for $|\varphi_l| < \varphi_l$ and $|G_{u_a u_a}| > |G_{u_a u_c}|$.

Four Particles/Unit Cell. Next, we consider a larger linear unit cell of four nanoparticles separated by a distance $R = \frac{d}{4}$. For this system, generally, $G(q)$ in the base $(A, C, B, D)$ is...
This is equivalent to the Hamiltonian of the SSH4 model (eq 9) with hoppings given by eq 25. As we see, this matrix is block-antidiagonal, i.e., sublattice symmetric. This is because there are two sublattices (odd and even sites) with only intersublattice connections. This symmetry protects the edge states on the central gap, fixing them at $q_{\text{edge}}$. These edge states are indistinguishable from the SSH model ones. However, SSH4 chains can also host edge states in the lower/upper gaps that lie in the same or opposite contour line. True or hidden mirror/inversion symmetries quantize the Zak phase of all gaps. The Zak phase for all the gaps, which represent the existence of edge states in each gap. In panel (f) we map the module of the dipoles for the edge states in the central and lower gaps.

As we see, the former respects the sublattice symmetry and is localized only in odd or even sublattices, while the latter has only zero weight in one of the sublattices.

Interestingly, due to accidental symmetries, in this system we can also recover the topology of the SSH model. When $G_{u} = G_{u}$ and $G_{u} = G_{u}$, or equivalently, $t = v$ and $\alpha = \omega$ in Figure 1(c), upper and lower gaps close and we have an analogue of the SSH model. Even when the period of the real unit cell is 4R, the effective tight binding unit cell has a period of 2R.

In Figure 4 we show a plasmonic analogue of the SSH4 model with $a = 12.5 \text{ nm}$, $d = 15a$, and $R = \frac{\pi}{4} = 3.75a$. By fixing the direction of the nanoparticles in sites $B$ and $D$ and rotating $A$ and $C$ as $\varphi = \left[ -\varphi, -\frac{\varphi}{2}, \varphi, \frac{\varphi}{2} \right] = -\frac{\varphi}{2}$, with $\varphi$ ranging from $-\frac{\pi}{4}$ (left unit cell in Figure 5(a)) to $\frac{\pi}{4}$ (right unit cell), a topological transition occurs at $\varphi = 0$ (middle unit cell), where the gap closes due to all $G_{u}$ being equivalent, as in the SSH model for $\upsilon = \omega$ (middle unit cell in panel (b)). In this system there’s also a transition from an inversion symmetric

\[
\begin{pmatrix}
0 & 0 & G_{u},u_{1} & G_{u},u_{1},e^{\imath q_{\text{edge}}} \\
0 & 0 & G_{u},u_{1} & G_{u},u_{1} \\
G_{u},u_{1} & G_{u},u_{2} & 0 & 0 \\
G_{u},u_{1},e^{\imath q_{\text{edge}}} & G_{u},u_{2} & 0 & 0
\end{pmatrix}
\]
Figure 5. Plasmonic analogue of the SSH model. Periodic chain of four prolate silver nanospheroids per unit cell, with long spheroidal axes forming angles with the chain direction $\varphi = \varphi_c = \frac{\pi}{4}$ and $\varphi_l = -\varphi_r = \varphi$ let free. The dimensions of the nanoparticles are $a = 12.5 \text{ nm}$ and $b = c = 0.4 a = 5 \text{ nm}$, and the interparticle distance is $R = \frac{2}{3} = 3.75a$. (a) Unit cells for $\varphi = \frac{\pi}{4}$, $0$, $\frac{\pi}{4}$. (b) Equivalent tight binding unit cells; the effective unit cells are dimeric, as in the SSH model. Solid and dashed black lines represent strong and weak bonds. (c) Plasmonic bands of the periodic system. Solid curves represent the bands for $\varphi = \pm \frac{\pi}{4}$, while dashed ones represent the bands for $\varphi = 0$, at the gap closing. (d) Plasmonic spectrum of a finite chain of 100 nanoparticles (25 unit cells). Bulk states are represented by blue lines, while red lines represent the pair of edge states, that appear after the gap closing at $\varphi = 0$. Red dot marks the values corresponding to the edge state plotted in panel (f). (e) Zak phase of central gap, which matches the number of edge states in panel (d). (f) Edge state for $\varphi = \frac{\pi}{4}$. The gradients represent the module of the dipoles in absence of incident field. Due to sublattice symmetry, the left edge state is localized at odd sublattices (A and C), while the right edge state is localized at even sublattices (B and D).

In the next section we will study how these edge states are excited by an incident electric field, depending on its polarization.

### SWITCHING EDGE STATES BY INCOMING ELECTRIC FIELD

A difference between electronics and plasmonics is that plasmons are not Fermions, so the bands are not naturally half-filled. In photonics, we need an incident field that overlaps spatially with the eigensolutions of the array. Once the incident field is fixed, by inverting eq 12, the dipoles of the chain are given by

$$ P = \left( G(\omega) - \frac{1}{\alpha(\omega)} I \right)^{-1} E_{\text{inc}}(\omega, t) $$

where $E_{\text{inc}}$ is a vector of the projections of the electric field in the directions of the major axes of the nanoparticles. Such projections are key in order to excite or not excite the protected states. When all the particles in the array are spherical or oriented in the same direction, the electric fields affect almost equally all the nanoparticles. However, when nanoparticles are oriented in different directions, some spatial symmetries are broken, affecting how an incident electric field couples to the edge states and allowing switching.

Plasmonic nanoparticle chain edge states are difficult to observe in experiments mainly due to the small dimension needed to avoid detrimental long-range effects. Despite these difficulties, they have been experimentally probed by near-field27,48 and far-field90 imaging techniques.

Let us analyze what happens when we excite the edge states of the plasmonic chains. In Figure 6 we plot the dipolar response to a linearly polarized electric field at normal incidence, depending on its polarization:

$$ E_{\text{inc}}(\omega, t) \propto \begin{pmatrix} \cos \eta \\ \sin \eta \\ 0 \end{pmatrix} $$

where $\eta$ is the angle of polarization of the electric field with respect to the $x$ axis. In order for the field to resonate with the nanoparticles and with the edge state mode, due to the losses of the nanoparticles, we need the incoming electric field to have the frequency of the edge state and a finite lifetime, that is, a pulse.

In Figure 6a–d, we analyze the edge states of the central gap, which are protected by chiral symmetry. In panels (e)–(h) we excite the edge states in the lower gap of the SSH4 chain, which are 4-way-chiral-symmetric. For both types, we consider chains with mirror, inversion, accidental mirror, and
Excitation of edge states of different plasmonic chains by an incoming linearly polarized electric field at normal incidence, depending on its angle of polarization $\eta$. We plot the module of dipolar moments at each site $p_{\alpha}$ normalized by its maximum value for all polarizations and sites. We use red and green gradients for chiral (central gap) in panels (a)–(d) and generalized 4-way chiral (lower gap) edge states in panels (e)–(h). As insets, we plot the spectra of the chains, where blue, red, and green dots represent bulk states, central gap edge states, and lower/upper gap edge states. (a) Mirror symmetric unit cell (see Figure 5), $q_\eta = \frac{\pi}{4}(-1, -1, 1, 1)$. The chain breaks the inversion symmetry, while incident electric field breaks mirror symmetry (except for $\eta = 0$ and $\eta = \pi$), allowing to switch off left or right edge states separately for $\eta \sim \frac{\pi}{4}$ and $\eta \sim \frac{3\pi}{4}$. Then, when applying a circular incident electric field, edge states bounce back and forth between the edges. (b) Inversion symmetric unit cell, $q_\eta = \frac{\pi}{4}(0, \frac{\pi}{2}, \frac{\pi}{2}, 0)$. Electric field does not break inversion symmetry, but allows to switch on and off both edge states simultaneously. (c) Accidentally mirror symmetric unit cell, $q_\eta = \left[\frac{\pi}{4}, \frac{\pi}{4}, \frac{\pi}{4}, \frac{\pi}{4}\right]$. As both true mirror and inversion symmetries are broken, both the amplitude and phase of the excited edge states differ. (d) Nonspatial-symmetric unit cell, $q_\eta = \frac{\pi}{4}(0, \frac{\pi}{2}, \frac{\pi}{2}, 0)$. As left–right edge states are still degenerate due to chiral symmetry, we have a response for both edges similar to case (c). (e) Mirror symmetric unit cell, $q_\eta = \left[\frac{\pi}{4}, \frac{\pi}{4}, \frac{\pi}{4}, \frac{\pi}{4}\right]$. (f) Inversion symmetric unit cell, $q_\eta = \left[\frac{\pi}{4}, \frac{\pi}{4}, \frac{\pi}{4}, \frac{\pi}{4}\right]$. (g) Accidentally mirror symmetric unit cell, $q_\eta = \left[\frac{\pi}{4}, \frac{\pi}{4}, \frac{\pi}{4}, \frac{\pi}{4}\right]$. (h) Nonspatial-symmetric unit cell, $q_\eta = \left[0, \frac{\pi}{2}, \frac{\pi}{2}, 0, 0.8\pi\right]$. Due to the absence of symmetries, left and right edge states are not degenerate and can be excited separately.

no spatial symmetries to see how this affects the optical response.

In Figure 6a we see the response of the SSH nanospheroid chain with mirror symmetry and $q_\eta = \frac{\pi}{4}(-1, -1, 1, 1)$ to a linearly polarized electric field at the frequency of the surface plasmon $\omega_{p\nu}$, depending on its polarization. Since all the nanoparticles are oriented at diagonals when the field is polarized in $x$ or $y$ directions ($\eta = 0, \frac{\pi}{2}$), all the particles are equally perturbed so mirror symmetry holds and left and right edge states are identical.

However, when we apply an electric field oriented at $\eta \neq 0, \frac{\pi}{2}$, the interaction with the external field depends on the nanoparticle. The sublattice symmetry is still preserved, as we see in Figure 6a. However, the external field breaks the mirror symmetry, allowing to have a different response at left and right edges. For $\eta \approx \frac{\pi}{4}$, the dipolar response is localized only at the left (right) edge. Then, by changing the polarization of the field, we can select left, right, or both edge states with the same or different weight.

Now if we apply a circularly polarized electric field at normal incidence, this is

$$E_{\nu\nu}(\omega, t) \propto \begin{pmatrix} \cos(\eta(t)) \\ \sin(\eta(t)) \\ 0 \end{pmatrix}$$

The nanospheroids convert the circular polarization of the incoming field to linear polarization. Then, the oscillations in left and right edges are not in phase, so the edge states “bounce back and forth” between left and right edges. Over a period $T$, the response of the chain loops two times over the $\eta$ axis in Figure 6a.
However, when the chain is inversion-symmetric, for example, the one in panel (b) \( \left( \varphi_e = \frac{\pi}{10} + \left[ 0, \frac{\pi}{2}, \frac{\pi}{3}, 0 \right] \right) \), the electric field preserves this symmetry, so the response in both edges is the same. We can switch on/off both edge states simultaneously. If the electric field is circularly polarized, then the oscillations in both edges are in phase.

When the chain is accidentally mirror-symmetric (panel (c), \( \varphi_e = \left[ \frac{4\pi}{9}, \frac{\pi}{2}, \frac{\pi}{3}, \frac{4\pi}{9} \right] \)), or has no spatial symmetries (panel (d), \( \varphi_e = \frac{\pi}{20} + \left[ 0, \frac{\pi}{2}, \frac{\pi}{3}, 0 \right] \)), the field couples more intensely to one of the edges. If we apply a circularly polarized electric field, the oscillations in the edges would not be just dephased as the bouncing states in the mirror symmetry chain, but they would differ also in amplitude.

For the edge states in lower (or upper) gaps, however, we find a different scenario. In a mirror symmetric SSH4 chain (panel (e), \( \varphi_e = \left[ \frac{4\pi}{9}, \frac{\pi}{2}, \frac{\pi}{3}, \frac{4\pi}{9} \right] \)), the external field does not appear to break the symmetry between edges. This may be due to the coexistence of generalized chiral symmetry and spatial symmetries. This means that we cannot select right or left edges. If the field is circularly polarized, then the oscillations in both edges are in phase. The same occurs for an inversion-symmetric unit cell (panel (f), \( \varphi_e = \left[ 0, \frac{\pi}{2}, \frac{\pi}{3}, 0 \right] \)) and in the accidentally symmetric case (panel (g), \( \varphi_e = \left[ 0, \frac{\pi}{2}, \frac{\pi}{3}, 0.71\pi \right] \)).

Finally, if the SSH4 unit cell has no spatial symmetries (panel (h), \( \varphi_e = \left[ 0, \frac{\pi}{2}, \frac{\pi}{3}, 0.8\pi \right] \)), left and right lower/upper gap edge states are no longer degenerate, so we can excite them separately at different frequencies. Due to the breaking of the degeneracy, these edge states may be more easily pushed out of the gap by disorder and hybridize with bulk states.

As we see, by orienting elongated nanoparticles, we have gained control in edge states, making possible to switch them off, select left, right, both, or bouncing edge states. This is not feasible in the nanosphere chain, as each single particle has an isotropic response for all the polarizations of the electric field. Here we have studied equidistant chains to show a gap can be opened by orientation in an otherwise gapless system; however, this degree of freedom can be exploited in more complex arrays. The extension to 2D lattices will lead to more interesting effects.

## CONCLUSIONS

In previous years, there have been several proposals to mimic topological electronic systems in photonics. Periodic arrays of metallic nanoparticles are an interesting platform to study topology in nanophotonics due to their plasmonic resonances in the visible range and their tunability. Here we have proposed means to open a topological gap not by rearranging the nanoparticles in an array as in crystalline topological electronic systems, but by orienting elongated particles. By adding this degree of freedom, we can mimic topological chains as the SSH model or its greater unit cell extensions in an equidistant array. The spatial polarization modulation allows also to switch on/off or select right, left, or bouncing edges states, by changing the polarization of the incoming electric field, as in the zigzag plasmonic chain. However, orientation of elongated nanoparticles in arrays also makes possible the suppression of the interaction between nanoparticles, to control and engineer spatial symmetries and filter modes. This opens a path toward exploiting features of nanoparticles for topology without a counterpart in condensed matter systems.

## ASSOCIATED CONTENT

### Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsphotonics.2c01526.

Polarizability of metallic nanospheres and nanospheres, and Green dyadic’s function projection (PDF)

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