Coupling and guided propagation along parallel chains of plasmonic nanoparticles

Andrea Alù\textsuperscript{1,5}, Pavel A Belov\textsuperscript{2,3} and Nader Engheta\textsuperscript{4}

\textsuperscript{1} Department of Electrical and Computer Engineering, The University of Texas at Austin, Austin, TX 78712, USA
\textsuperscript{2} Department of Electronic Engineering, Queen Mary University of London, Mile End Road, London E1 4NS, UK
\textsuperscript{3} Department of Photonics and Optoinformatics, St Petersburg State University of Fine Mechanics and Optics Kronverksky Pr. 49, 197101, St Petersburg, Russia
\textsuperscript{4} Department of Electrical and Systems Engineering, University of Pennsylvania, 200 South 33rd Street—ESE 203 Moore, Philadelphia, PA 19104, USA
E-mail: alu@mail.utexas.edu

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**Abstract.** We derive a dynamic closed-form dispersion relation for the analysis of the entire spectrum of guided wave propagation along coupled parallel linear arrays of plasmonic nanoparticles, operating as optical ‘two-line’ waveguides. Compared to linear arrays of nanoparticles, our results suggest that these waveguides may support more confined beams with comparable or even longer propagation lengths, operating analogously to transmission-line segments at lower frequencies. Our formulation fully takes into account the entire dynamic interaction among the infinite number of nanoparticles composing the parallel arrays, considering also the realistic presence of losses and the frequency dispersion of the involved plasmonic materials, providing physical insights into the guidance properties that characterize this geometry.

\textsuperscript{5} Author to whom any correspondence should be addressed.
1. Introduction

Linear chains of plasmonic (silver or gold) nanoparticles have been suggested to be used as optical waveguides in several recent papers [1]–[11]. Owing to the design flexibility and the relatively greater easiness of construction within current nanotechnology, the realization of such ultracompact waveguides has been thoroughly studied and analyzed over the last few years. However, recent experimental realizations of such devices at the nanoscale have revealed problems due to the strong sensitivity to material absorption and to inherent disorder. The guided beam cannot usually travel longer than a few nanoparticles before its amplitude is lost in the noise. This is mainly because linear arrays of small nanoparticles have the property of concentrating the optical energy in a sub-wavelength region of space, in large part filled by lossy metal. If this is indeed appealing in terms of power concentration and for enhancing the nanoscale interaction with light, it also has the clear disadvantage of strong sensitivity to material and radiation losses. In general, there is a well-known trade-off between energy concentration and confinement and robustness to loss in several plasmonic waveguide geometries [12]. As we have noted in [13], a bare conducting wire at low frequencies has analogous limitations: although metals are much more conductive and less lossy in radiofrequencies, connecting two points in a regular circuit with a single wire would still produce unwanted spurious radiation and sensitivity to metal absorption. This problem, which is much amplified at optical frequencies due to the poorer conductivity and higher loss of metals in the visible, is simply approached at low frequencies by closely pairing two parallel wires (or, which is the same, placing a ground plane underneath the conducting trace), forming the well-known concept of a transmission line that provides a return path for the conduction current. Analogously, applying the nanocircuit concepts [14, 15], we have recently put forward ideas to realize optical nanotransmission-line waveguides in different geometries [16, 17], which have been proved to be more robust to material and radiation losses and may provide a wider bandwidth of operation. In particular, one such idea consists in pairing together two parallel arrays of plasmonic nanoparticles, suggesting that the coupling among the guided modes may improve the guidance performance. In [13], we have shown that this is indeed the case: operating with the antisymmetric longitudinal mode, such parallel chains may indeed confine the beam in the background region between the chains, leading to large power confinement without significantly affecting the robustness to material absorption and radiation losses as compared to the isolated array scenario. In particular, we have shown that operating with these modes near
Figure 1. Geometry of the problem: a pair of linear arrays of plasmonic nanoparticles as an optical two-line waveguide. The sketch reports the polarization properties of quasi-longitudinal modes with symmetric and antisymmetric properties.

the light line would, in many senses, lead to operation close to a regular transmission line at low frequencies, but available in the visible regime.

Here, we present a complete, closed-form dynamic solution for the dispersion of the eigenmodes supported by parallel chains, fully taking into account the coupling among the infinite number of particles composing the two-chain array, even in the presence of material absorption, radiation losses and frequency dispersion. This derivation allows us to discuss the complete spectrum of guided modes supported by this geometry and analyze the differences between various polarizations and the analogies to the isolated chain geometry. The results confirm the validity of the analogy between these parallel arrays of nanoparticles and optical transmission lines, and they provide further insights into the operation and the large spectrum of modes guided by these paired arrays of nanoparticles. Applications for low-loss optical communications, optical switching, nonlinearity enhancement and sub-wavelength imaging devices are envisioned.

2. Dispersion relations for guided propagation

Consider the geometry of figure 1, i.e. two identical linear arrays of plasmonic nanoparticles with radius \( a \), period \( d > 2a \) and interchain distance \( l > d \). This geometry has been preliminarily analyzed in [13] for its longitudinally polarized antisymmetric guided modes, where it was shown that the coupling between the chains, limited in that analysis to its dominant contribution coming from the averaged current density on the chain axes, was expected to generate the splitting of the regular longitudinal mode guided by an individual linear array into two coexisting longitudinal modes, respectively, with symmetric and antisymmetric field distributions and polarization properties, as sketched in figure 1. The antisymmetric mode is the...
one corresponding to transmission-line operation [13], as outlined in the introduction, for which two antiparallel displacement current flows are supported by the parallel chains. A similar modal propagation has been analyzed in [7] for a related distinct geometry, consisting of longitudinal dipoles placed over a perfectly conducting plane. Also our analysis of quadrupolar chains [17] may, in the limit of $l \to 0$, have some analogies to this antisymmetric operation. In the following, we rigorously approach the general problem of modal dispersion along the parallel chains of figure 1, extending our general analysis in [10] valid for one isolated chain. Our formulation fully takes into account the entire coupling among the infinite nanoparticles composing the pair of arrays and the possible presence of material absorption, radiation losses and frequency dispersion.

We model each nanoparticle in the coupled array of figure 1 as a polarizable dipole with polarizability $\alpha$, an assumption that is valid as long as $\alpha \ll \lambda_b$, with $\lambda_b$ being the wavelength of operation in the background material. For simplicity, we assume a scalar polarizability, implying that the particles are isotropic (nanospheres, easy to realize as colloidal metal particles) or, for more general shapes, focusing on one specific field polarization. It is relevant to stress that the dipolar approximation represents a good assumption for small nanoparticles, and in particular for nanospheres, because of their inherent symmetries. We have verified that this approximation holds very well even in the limit of very small gaps, as those considered in the following examples [10]. The use of additional multipolar orders, as considered, e.g., in [18], may increase the accuracy of the calculation, but also complicate some of the physical insights outlined in the following.

We assume an $e^{-i\omega t}$ time convention in the rest of this paper.

For a single isolated chain, the spectrum of supported eigenmodes may be split into longitudinal and transverse polarization with respect to the chain axis $\hat{x}$ [10]. In particular, for $e^{i\beta z}$ propagation, the corresponding guided wavenumber $\beta$ satisfies the following closed-form dispersion relations, respectively, for longitudinal and transverse modes:

$$
L = 3\tilde{d}^{-3}f_3(\tilde{\beta}, \tilde{d}) - i\tilde{d} f_2(\tilde{\beta}, \tilde{d}) - \alpha^{-1} = 0,
$$

$$
T = -\frac{3}{2}\tilde{d}^{-3}f_3(\tilde{\beta}, \tilde{d}) - i\tilde{d} f_2(\tilde{\beta}, \tilde{d}) - \tilde{d}^2 f_1(\tilde{\beta}, \tilde{d}) - \alpha^{-1} = 0,
$$

where $f_N(\tilde{\beta}, \tilde{d}) = \text{Li}_N(e^{i(\beta + 1)d}) + \text{Li}_N(e^{-i(\beta - 1)d})$, and

$$
\text{Li}_N(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^N}
$$

is a polylogarithm function of order $N$ [19] and all the quantities have been normalized, consistent with [10], as $\tilde{d} = k_b d$, $\tilde{\beta} = \beta / k_b$ and $\tilde{\alpha} = k_b^3 \alpha / (6\pi \varepsilon_b)$, with $k_b = 2\pi / \lambda_b$ being the background wavenumber and $\varepsilon_b$ the corresponding permittivity.

These equations fully take into account the dynamic coupling among the infinite number of particles composing the linear chain. They are real valued for lossless particles (for which $\text{Im}[\tilde{\alpha}^{-1}] = -1$ [10]), supporting guided modes with $\tilde{\beta} > 1$, but they are also fully valid in the complex domain when realistic material losses are considered, making it possible to evaluate the realistic damping factors associated with material absorption and radiation losses. They can be also applied to the leaky-wave modal regime, for which $\text{Re}[\tilde{\beta}] < 1$ and the chain radiates as an antenna in the background region [20].

When $l$ is finite in figure 1, i.e. there are two parallel chains, their mutual coupling produces a modification of their guidance properties, which may be taken into account by considering the...
polarization fields induced by the electric field from each chain on the other. The fields radiated by each chain may be expanded into cylindrical waves, allowing us to write the general closed-form expressions for the coupling coefficients between the two chains.

Without loss of generality, we can assume that the particles composing the first chain, located at \( y = 0 \), are polarized by an eigenmodal wave with dipole moments \( p_1 e^{i \beta m d} \), where \( m \in \mathbb{Z} \) is the integer index for each nanoparticle of the chain. The equivalent current distribution on the \( x \)-axis may be written as

\[
J(x) = -i \omega p_1 \sum_{m=-\infty}^{\infty} e^{i \beta m d} \delta(x - md),
\]

where \( \delta(\cdot) \) is the Dirac delta function. The fields radiated by such a current distribution may be expanded into cylindrical waves and may be used to evaluate the coupling coefficients between one chain and the other, with dipole moments \( p_2 e^{i \beta m d} \) located at \( y = l \), yielding

\[
C_{xx} = -\frac{3}{d} \sum_{m=-\infty}^{\infty} \tilde{b}_m^2 K_0[\tilde{b}_m l],
C_{xy} = C_{yx} = -\frac{3i}{d} \sum_{m=-\infty}^{\infty} \sqrt{\tilde{b}_m^2 + 1} \tilde{b}_m K_1[\tilde{b}_m l],
C_{yy} = \frac{3}{l d} \sum_{m=-\infty}^{\infty} (\tilde{b}_m^2 + 1) \tilde{b}_m K_0[\tilde{b}_m l] + \tilde{b}_m K_1[\tilde{b}_m l],
C_{zz} = \frac{3}{2d} \sum_{m=-\infty}^{\infty} (\tilde{b}_m^2 + 2) K_0[\tilde{b}_m l] - \tilde{b}_m^2 K_2[\tilde{b}_m l],
C_{xz} = C_{zx} = C_{yz} = C_{zy} = 0,
\]

where \( \tilde{b}_m = \sqrt{\beta + (2\pi m/d)^2} - 1 \) and \( K_m[\cdot] \) are the modified Bessel functions of the order of \( m \) and \( l = kd l \). The generic coupling coefficient \( C_{ij} \) expresses the polarization along \( j \) on one chain induced by the \( i \)-polarized dipoles on the other chain. The summations in (3) have very fast convergence, and the dominant term \( (m = 0) \) is usually sufficient to take into account the dominant contribution to the coupling, an approximation that is consistent with the approach we used in [13]. The numerical results shown in the following sections have been obtained by considering the first ten terms in the summations (3), even though full convergence has been usually achieved after the first one or two terms. The form of the coupling coefficients in (3) ensures that longitudinal (directed along \( x \)) and transverse modes polarized along \( y \) are coupled through \( C_{xy} \), whereas transverse modes polarized along \( z \) are not coupled with the orthogonal polarizations.

The complete closed-form dispersion relation for the eigenmodes supported by the parallel chains may be written as

\[
\begin{vmatrix}
L & 0 & C_{xx} & C_{xy} \\
0 & T & C_{xy} & C_{yy} \\
C_{xx} & -C_{xy} & L & 0 \\
-C_{xy} & C_{yy} & 0 & T
\end{vmatrix} \begin{vmatrix}
T & C_{zz} \\
C_{zz} & T
\end{vmatrix} = 0
\]

or in a more compact form

\[
[(L \pm C_{xx}) (T \mp C_{yy}) + C_{xy}^2] (T \pm C_{zz}) = 0.
\]
The left-hand side of equation (5) consists of the product of two terms: the first determines the dispersion of the coupled modes polarized in the $xy$-plane (among which are the quasi-longitudinal antisymmetric modes considered in [13]), whereas the second determines the purely transverse modes polarized along $z$. This dispersion equation is completely general and fully takes into account the entire dynamic interaction among the infinite particles composing the two parallel chains. Since the coupling coefficients (3) tend rapidly to zero for increased $l$, equation (5) represents the perturbation of the original transverse and longitudinal modes supported by the two linear chains independently given by $L = 0$ and $T = 0$, respectively [10], produced by the coupling coefficients $C$. In particular, it is seen that each of the three orthogonal polarizations (along $x$, $y$, $z$) splits into two branches due to the coupling between the chains, one with symmetric and the other with antisymmetric properties (consistent with the sketch in figure 1), leading to six modal branches of guided modes, some of which are supported at the same frequency. In particular, the modes in the $xy$-plane are mixed together (i.e. the parallel chains do not support purely longitudinal or purely $y$-polarized modes, but they do support purely transverse $z$-polarized modes).

In the limit of lossless particles, since $L$ and $T$ are real for any $\bar{\beta} \gtrless 1$ [10], by inspecting equation (5) we note that the parallel chains still support lossless guided propagation for any $1 \leq \bar{\beta} \leq \pi/\bar{d}$. In the following, we analyze in detail the modal properties of this setup in its different regimes of operation.

3. Guided modes of parallel chains of silver nanospheres

In this section, we consider the different regimes of guided propagation supported by the parallel chains of figure 1, considering realistic optical materials composing the plasmonic nanoparticles. In the case of a chain of homogeneous spherical particles of radius $a$ and permittivity $\varepsilon = \varepsilon_r + i \varepsilon_i$, their normalized polarizability satisfies the following relations [10]:

\[
\begin{align*}
\text{Re}[\tilde{\alpha}^{-1}] &= \frac{3}{2} (k_b a)^{-3} \frac{\varepsilon_r + 2 \varepsilon_b}{\varepsilon_r - \varepsilon_b}, \\
\text{Im}[\tilde{\alpha}^{-1}] &= -1 - \frac{9 \varepsilon_i}{2} \left( \frac{\varepsilon_b (k_b a)^{-3}}{(\varepsilon_r - \varepsilon_b)^2 + \varepsilon_i^2} \right).
\end{align*}
\]

This polarizability model is analogous to the commonly used quasi-static polarizability definition for a small sphere, with the addition of radiation loss (as from the $-1$ term in Im[\tilde{\alpha}^{-1}]), to comply with energy conservation. Since the guided modes are perturbations of the longitudinal and transverse modes supported by the isolated chains, there is no need to analyze here again in full detail how variations in the chain geometry, i.e. in $a$, $d$ and/or the involved materials, may affect the guidance of the parallel chains, since we have already extensively studied how these changes affect the guidance of isolated chains in [10]. In the following, therefore, we focus on one specific realistic design of the chains and we employ the exact formulation developed in the previous section to characterize the modal properties of two of such parallel arrays coupled together. In the following, we focus on colloidal silver nanospheres embedded in a glass background ($\varepsilon_b = 2.38 \varepsilon_0$). We use experimental data available in the literature to model the silver permittivity at optical frequencies [23] and we assume $a = 10$ nm and $d = 21$ nm for the two chains. In general, we can predict that larger separation distances for the same particle size are expected to weaken the guidance properties of the array and reduce...
Figure 2. Modal dispersion for the quasi-longitudinal modes supported by two parallel chains with interchain distance $l = 50$ nm. The dispersions are compared with that of an isolated chain (thin solid line). The lighter blue shadowed region refers to leaky-wave propagation, whereas the darker orange region refers to the first Bragg stop band.
the bandwidth of operation and robustness to loss, whereas particles with larger size have the opposite effect.

3.1. Quasi-longitudinal propagation (forward modes)

An isolated linear chain of plasmonic nanoparticles supports forward-wave longitudinal guided modes (x-polarized), satisfying the dispersion relation \( L = 0 \), over the frequency regime for which

\[
6[\text{Ci}_3(h + \pi) + dh \text{Ci}_2(h + \pi)] < \frac{d^3}{3} \text{Re}[\alpha^{-1}] < 3[\xi(3) + \text{Ci}_3(2dh) + dh \text{Ci}_2(2dh)],
\]

where \( \text{Ci}_N(\theta) \) are Clausen’s functions \(^{19}\) and \( \xi(.) \) is the Riemann zeta function. For the case at hand (silver nanoparticles, \( a = 10 \text{ nm} \) and \( d = 21 \text{ nm} \)), such a modal regime is supported over a relatively wide range of frequencies between 550 and 850 THz, as shown in figure 2 (thin solid black line). In particular, in the figure we plot (a) the real and (b) the imaginary parts of the normalized \( \beta \) and (c) the propagation length, i.e. the distance traveled by the guided mode before its amplitude is \( e^{-1} \) of the original value, which is equal to \( \text{Im}[\beta]^{-1} \). The shadowed regions at the sides of the plots delimit the leaky-wave region (the left side, lighter blue shadowed region), for which \( \text{Re}[\beta] < 1 \) and the mode radiates in the background region \(^{24}\), and the stop-band region (the right side, darker shadow, brown), where \( \text{Re}[\beta] = \pi/d \) when lossless particles are considered and the mode is evanescent in nature. In between these two regions, as defined by equation (7), the modes are guided and \( \text{Im}[\beta] \), i.e. the damping factor, is only associated with material losses, because in the limit of lossless particles the mode would not radiate and \( \text{Im}[\beta] = 0 \). In the leaky-wave region (lighter blue shadow) the damping is larger, due to additional radiation losses \(^{20}\), whereas in the stop band (darker shadow) the mode does not propagate and it is reflected back by the chain due to Bragg reflection (the ideal Bragg stop-band line \( \text{Re}[\beta] = \pi/d \) is shown in figure 2 as a thin pink line). Near the light line (\( \text{Re}[\beta] \approx 1 \)) the mode is poorly guided by an isolated chain, but its propagation length may reach relatively large values, about 1 \( \mu \text{m} \).

In the same figure, we plot the variation of these dispersion diagrams in the case of two coupled parallel chains separated by a finite distance \( l \). In this case, the longitudinal modes are coupled with each other, also polarizing the chains with a small transverse component along \( y \), consistent with the value of \( C_{xy} \). The longitudinal mode dispersion splits into two quasi-longitudinal branches, one with symmetric and the other with antisymmetric properties with respect to x-polarization (as sketched in figure 1). The two modes satisfy, respectively, the following dispersion relations, consistent with equation (5):

\[
\begin{align*}
\text{sym:} & \quad (L + C_{xx})(T - C_{yy}) + C_{xy}^2 = 0, \\
\text{antisym:} & \quad (L - C_{xx})(T + C_{yy}) + C_{xy}^2 = 0,
\end{align*}
\]

providing the following constraints on the polarization eigenvectors for the two chains (obtained by calculating the eigenvectors associated with equation (4)):

\[
\begin{align*}
\text{sym:} & \quad \begin{cases} \\
& \mathbf{p}_1 \cdot \hat{x} = \mathbf{p}_2 \cdot \hat{x}, \\
& \mathbf{p}_1 \cdot \hat{y} = -\mathbf{p}_2 \cdot \hat{y},
\end{cases} \\
\text{antisym:} & \quad \begin{cases} \\
& \mathbf{p}_1 \cdot \hat{x} = -\mathbf{p}_2 \cdot \hat{x}, \\
& \mathbf{p}_1 \cdot \hat{y} = \mathbf{p}_2 \cdot \hat{y}.
\end{cases}
\end{align*}
\]
Figure 3. Similarly to figure 2, modal dispersion for the quasi-longitudinal modes supported by two parallel chains with interchain distance $l = 30$ nm.
Figure 2 shows as a first example the dispersion of symmetric and antisymmetric modes for $l = 50$ nm. It is noted that the small coupling between the chains slightly perturbs the dispersion of the modes, causing the antisymmetric mode (blue dashed line, with polarization currents oppositely flowing along the chains) to have slightly larger real and imaginary parts of $\tilde{\beta}$ with respect to the unperturbed longitudinal mode supported by an isolated chain (light solid line) in the guided regime. Conversely, the symmetric mode (thick red solid line) supports slightly lower values of $\text{Re}[\tilde{\beta}]$. The perturbation is stronger near the light line and in the leaky-wave region, since the mode is less confined around each chain in this regime. The symmetric operation allows an increase in the propagation length of up to $1.5 \mu$m, since the coupling between the parallel chains with polarization currents flowing in the same direction can boost up the mode. On the other hand, the antisymmetric operation has slightly lower propagation lengths, but this is accompanied by the important advantage of much stronger field confinement, as we note in the following. The derivative $\partial \text{Re}[\tilde{\beta}] / \partial \omega > 0$ ensures that the modes supported in this regime are all forward wave, and this is also confirmed by the condition $\text{Im}[\tilde{\beta}] > 0$, which ensures that phase and group velocity are parallel to each other for both modes.

As an aside, it should be noted that in the leaky-wave region (blue lighter shadow on the left) the forward-wave modes are improper in nature [24], implying that the dominant cylindrical wave radiated by the chain grows with the distance from the chain instead of decaying. This implies that for a correct evaluation of the modal properties and the field distribution generated in this forward-leaky-mode regime, the formulae of equation (3) for the index $m = 0$ need to be corrected using the Hankel functions of second order instead of the modified $K_n$ functions.

Figure 3 shows analogous results for closer chains, with $l = 30$ nm. It is seen that the perturbation from the isolated chain is now stronger and the coupling between the modes generates some isolated resonant regions of stronger absorption, which are associated with stronger transversely polarized components of the field. Still, near the light line propagation lengths are relatively large.

Figure 4 shows the calculated orthogonal magnetic field distribution (snapshot in time) on the $xy$-plane for the modes supported by the chains of figure 3 ($l = 30$ nm) at the frequency $f = 585$ THz, near the light line. The figure emphasizes how the modal distribution is quite different in the three scenarios, even if the guided wavenumbers are similar. Figure 4(a) corresponds to antisymmetric propagation, for which the two chains support the eigenvector polarizations $\mathbf{p}_1 = \hat{x} + (0.14 i - 0.008)\hat{y}$ and $\mathbf{p}_2 = -\hat{x} + (0.14 i - 0.008)\hat{y}$, consistent with equation (9). The corresponding normalized wavenumber at this frequency is $\tilde{\beta}_{\text{ asym}} = 1.38 + i 0.1$. It can be seen how the magnetic field is very much confined in the tiny background region delimited by the two chains, similar to the field propagation in a regular transmission line at low frequencies. Also the electric field is mainly transverse in the region between the chains, supporting the transverse electromagnetic configuration, again typical of a transmission-line mode. This regime of operation, whose interesting properties we have already described in detail in [13], may lead to relatively low-loss optical guidance with ultraconfined properties in the space between the chains, similar to an optical nanotransmission line. This functionality may be particularly appealing for optical switching, nanoscale field interaction, sensing and nonlinearity enhancements.

Figure 4(b), on the other hand, refers to the symmetric mode for the same parallel chains. In this case, $\mathbf{p}_1 = \hat{x} + (0.08 i - 0.003)\hat{y}$, $\mathbf{p}_2 = \hat{x} - (0.08 i - 0.003)\hat{y}$ and $\tilde{\beta}_{\text{ sym}} = 1.13 + i 0.053$. The currents flowing along the chains are now parallel to each other, producing fields very much spread all around the outside background region and weak field concentration in between.
Figure 4. Magnetic field distribution (snapshot in time) for the chains of figure 3 at the frequency $f = 585$ THz: (a) antisymmetric mode, (b) symmetric mode and (c) isolated chain. All the plots are drawn with the same color scale bar (normalized to the modal amplitude on the left of the figure). The total length of the simulated region is $2\lambda_b$.

them. This operation is equivalent to two parallel current flows, leading to small fields in between them. A single linear chain has analogous guidance properties, shown in figure 4(c) (for comparison, in this third example the chain is positioned at the same location as the lower chain in the other two panels). In this case, the mode is purely longitudinal and $\tilde{\beta}_{\text{single}} = 1.18 + i 0.072$, implying weak guidance.

Comparing the three field plots (note that for fair comparison they have been calculated with the same color scale and under the same initial amplitude excitation), it becomes evident that the antisymmetric longitudinal operation allows for a much stronger confinement of the field, with comparable propagation length. By field confinement here, we consider the field decay away from the array axis, which is always of a higher rate for the antisymmetric longitudinal mode compared to an isolated chain or the symmetric mode. By increasing the distance between the chains, as in the examples of figure 2, we achieve similar confinement in the region between the chains with reduced attenuation. In addition to a quantitatively larger field confinement achieved with the antisymmetric mode (compared to the isolated chain, despite the larger transverse physical cross section of the parallel chain geometry), this operation ensures larger confinement in between the two chains, which is particularly appealing for applications aiming at enhancing the nanoscale optical interaction.
Figure 5. Similar to figure 4, magnetic field distribution (snapshot in time) for the chains of figure 3 at the frequency $f = 680$ THz: (a) antisymmetric mode, (b) symmetric mode and (c) isolated chain.

These properties are not only limited to the modes operating near the light line, but they are also valid for higher frequencies and more confined modes. For instance, in figure 5 we show the magnetic field plots for the same chains, operating at $f = 680$ THz. At these frequencies, as seen in figure 3, the three cases have similar levels of absorption and more confined slow-wave modes. The antisymmetric excitation is characterized in this case by $p_1 = \hat{x} + (0.37 i - 0.038)\hat{y}$, $p_2 = -\hat{x} + (0.37 i - 0.038)\hat{y}$ and $\beta_{\text{asym}} = 2.42 + i 0.091$. Its field distribution (figure 5(a)) still shows strong confinement between the two chains, where a ‘quasi-uniform’ magnetic field may propagate as if guided by a transmission line. The wave is slower than in the case of figure 4, due to increased Re[$\beta$], but the level of absorption is still quite good and the mode can propagate for over two wavelengths with no strong attenuation. The symmetric operation, for which $p_1 = \hat{x} - (0.158 i - 0.082)\hat{y}$, $p_2 = \hat{x} + (0.158 i - 0.082)\hat{y}$ and $\beta_{\text{sym}} = 1.9 + i 0.074$, once again provides worse field confinement, as expected. In this case (figure 5(b)) the field is spread around the chains and is very weak in the region between the two chains. Similar spreading is noticeable in the single isolated chain configuration of figure 5(c), with $\beta_{\text{single}} = 2.06 + i 0.077$. We note that the field spreading in the region around the chains would also be more sensitive to radiation losses produced by disorder and technological imperfections. This is consistent with our findings in [11], in which we have quantitatively modeled the possible presence of disorder along such periodic arrays in terms of effective additional loss in the polarizability coefficient. We predict that the antisymmetric transmission-line operation of the parallel chains
may produce more robust optical guidance confined in the region between the chains compared to the symmetric operation or the isolated chain.

From the previous examples, it is evident that in this regime the modes guided by the parallel chains are quasi-longitudinal with a spurious transverse polarization, arising from the coupling, which is nearly 90° out of phase with respect to the longitudinal polarization. In figure 6, for the parallel chains of figures 2 and 3 we have calculated the level of transverse cross-polarization (defined as the ratio of the longitudinal to the transverse component of $\mathbf{p}$) induced on the particles due to coupling, as a function of frequency. It is evident that its level increases for closer chains, as expected, and it is larger for antisymmetric modes. In the region of enhanced absorption that we have noted in figure 3, the corresponding level of cross-polarization is also very high, implying that at some resonance frequencies the transverse polarization may be even higher than the longitudinal one, noticeably affecting the chain guidance. As expected, in these regimes the losses are inherently larger. The coupling is minimal near the light line and in the leaky-wave and stop-band regimes, and reaches its maximum somewhere inside the guidance region, whose position in frequency varies depending on the distance between the chains and the mode of operation.

3.2. Quasi-transverse y-polarized propagation (backward modes)

We have discussed in [10] that a single isolated linear chain may also support transversely polarized guided modes, satisfying the exact dispersion relation $T = 0$. In this case, the condition on the particle polarizability is

$$\ddot{d}^{3} \tilde{\alpha}_{\text{min}}^{-1} \ddot{d}^{3} \text{Re}[\tilde{\alpha}^{-1}] < -3[C l_{3}(\ddot{d} + \pi) + \ddot{d} C l_{2}(\ddot{d} + \pi) - \ddot{d}^{2} C l_{1}(\ddot{d} + \pi)],$$

(10)
Figure 7. Analogous to figure 2, modal dispersion for the quasi-transverse $y$-polarized modes supported by two parallel chains with interchain distance $l = 50$ nm. In the antisymmetric polarization, as well as in the isolated chain, the presence of a second quasi-transverse mode with weakly guided properties is evident, explaining the presence of two distinct branches.
Figure 8. Polarization properties of the symmetric and antisymmetric quasi-transverse modes supported by parallel chains as in figure 1.

where $\alpha^{-1}_\text{min}$ has been defined in [10]. In this regime the isolated chain always supports two distinct modes at the same frequency, both with the same transverse polarization: one is guided along the chain and has backward-wave properties and the other is weakly guided, with forward-wave properties and $\text{Re}[\beta] \simeq 1$ (this eigenmode is basically a simple plane wave traveling in the background region, weakly polarizing the nanoparticles. This is not of interest for guidance purposes [10], but it is still discussed here for the sake of completeness). For the geometry at hand, transversely polarized propagation is supported over the frequencies between 650 and 800 THz, in part overlapping with the longitudinally polarized regime, as shown in figure 7 (thin black line), consistent with equation (10). Remarkable differences are noted between longitudinal and transverse polarization: the confined transverse mode is backward in nature, explaining the negative slope of $\text{Re}[\beta]$ versus frequency and the negative sign of $\text{Im}[\beta]$. Correspondingly, the bandwidth is more limited and losses are higher, as is usually the case for backward-wave waveguides. As a consequence, the leaky-wave operation arises now at the upper boundary of the guided regime (lighter shadowed region in figure 7) [20], whereas the Bragg stop band is positioned at the lower end of the guidance band (darker shadow).

Due to modal coupling in the $xy$-plane, when the coupling between parallel chains is considered, the quasi-transverse modes still satisfy the dispersion relations (8) and the polarization eigenvectors obey the same relations (9). It should be noted, however, that in this regime the modes are quasi-transverse and therefore the antisymmetric mode now corresponds to parallel $y$-polarized chains, whereas the symmetric mode supports antiparallel polarization along $y$, consistent with (9), as sketched in figure 8.

Figure 7 shows the dispersion of symmetric and antisymmetric quasi-transverse modes for $l = 50$ nm. Once again, the relatively small coupling between the chains produces a minor perturbation of the original backward-wave purely transverse mode, which causes the antisymmetric mode to have slightly lower real and slightly larger imaginary parts of $\beta$. Conversely, the symmetric mode supports slightly larger values of $\text{Re}[\beta]$. As in the previous section, the coupling is stronger near the light line and in the leaky-wave region (lighter shadow), as expected. Also in this scenario the symmetric operation allows longer propagation lengths, even if in this case the $y$-polarized currents are oppositely oriented (see figure 8).

Compared to quasi-longitudinal forward modes, the propagation length is significantly reduced for these confined modes, due to the backward-wave nature of these modes and their transverse polarization. Of course, following the results in [10], the propagation length may be somewhat increased and optimized by increasing the size of the nanoparticles and/or reducing the interparticle distance $d$. Compared to the backward mode supported by isolated chains, these
Similarly to figure 7, modal dispersion for the quasi-transverse \( y \)-polarized modes supported by two parallel chains with interchain distance \( l = 30 \text{ nm} \).

Results show that the coupling between two parallel chains may increase the propagation length of backward-wave optical nanowaveguides, simultaneously improving their field confinement in the space between the two lines, which may be of interest for several applications.
Figure 10. Magnetic field distribution (snapshot in time) for the chains of figure 9 at the frequency \( f = 700 \text{ THz} \): (a) antisymmetric mode, (b) symmetric mode and (c) isolated chain.

Figure 9 shows analogous results in the case of closer chains \((l = 30 \text{ nm})\). Also in this case, the perturbation from the isolated chain is stronger and the bandwidth of backward operation may be increased by using two parallel chains in the symmetric mode. Here leaky modes (lighter shadow) are proper in nature and therefore equations (3) also apply to this regime in the way they are written. Both in figures 7 and 9, for completeness, we also show the modal branch associated with the weakly guided forward-wave transverse mode, which is visible very close to the light line (thin solid line very close to the \( \text{Re}[\bar{\beta}] = 1 \) line in both plots). Consistent with its forward-wave properties, \( \text{Im}[\bar{\beta}] > 0 \) for this mode. As outlined above, this mode is of minor interest for guidance purposes, since it is a minor perturbation of a plane wave traveling in the background region, very weakly affected by the presence of the chains. It is noted, as expected, that this second branch is present only for the antisymmetric modes, whose \( y \)-polarization is in the same direction for both chains. Indeed, in figures 7 and 9 one can see a second branch for the blue dashed lines, near the light line, corresponding to the weakly guided forward mode traveling in the background (not of interest here).

Figure 10 shows the magnetic field for these backward-wave modes as in figure 9 at the frequency \( f = 700 \text{ THz} \). In the antisymmetric case (figure 10(a)) \( p_1 = (0.076 - 0.12i)\hat{x} + \hat{y}, \ p_2 = -(0.076 - 0.12i)\hat{x} + \hat{y} \) and \( \bar{\beta}_{\text{asym}} = 3.95 - 0.46 \); in the symmetric case \( p_1 = (0.02 - 0.016i)\hat{x} - \hat{y}, \ p_2 = (0.02 - 0.016i)\hat{x} + \hat{y} \) and \( \bar{\beta}_{\text{sym}} = 5.88 - 0.72 \); for the isolated chain \( \bar{\beta}_{\text{single}} = 5.036 - 0.42 \). The field distributions in some sense resemble the one for quasi-longitudinal modes, but the presence of a dominant transverse polarization does not allow an analogous strong transmission-line confinement in this backward-wave regime for the
Figure 11. Amplitude of the longitudinal cross-polarization for the chains of figures 7 and 9, operating in the quasi-transverse regime.

antisymmetric modes. Still, the plots confirm that relatively long backward-wave propagation (over one wavelength) is achievable using coupled parallel chains.

Figure 11 shows the level of longitudinal cross-polarization for the chains of figures 7 and 9. In this scenario, the cross-polarization is in general lower than for quasi-longitudinal modes and it is stronger for symmetric modes. Once again, the cross-polarization is stronger for closely coupled chains and it has some resonant peaks in the middle of the guidance region, for which the damping is correspondingly increased.

3.3. Purely transverse z-polarized propagation (backward modes)

When the chains are polarized along $\hat{z}$ the supported modes are purely transverse, consistent with (4). Due to symmetry, the properties for isolated chains are identical to those described in the previous section, and therefore here we discuss how the coupling may have a different effect on the backward-wave guidance properties in this polarization. The coupling coefficient $C_{zz}$ splits the transverse modal branch of propagation into two modes, with dispersion relations:

\begin{align}
\text{sym:} & \quad T + C_{zz} = 0, \\
\text{antisym:} & \quad T - C_{zz} = 0
\end{align}

providing the following constraints on the polarization eigenvectors for the two chains:

\begin{align}
\text{sym:} & \quad \mathbf{p}_1 \cdot \hat{z} = \mathbf{p}_2 \cdot \hat{z}, \\
\text{antisym:} & \quad \mathbf{p}_1 \cdot \hat{z} = -\mathbf{p}_2 \cdot \hat{z}
\end{align}
Figure 12. Analogous to figures 2 and 7, modal dispersion for the quasi-transverse \( z \)-polarized modes supported by two parallel chains with interchain distance \( l = 50 \) nm.
Figure 13. Similarly to figure 12, modal dispersion for the quasi-transverse $z$-polarized modes supported by two parallel chains with interchain distance $l = 30 \text{ nm}$.
Figure 14. Electric field distribution (snapshot in time) for the chains of figure 12 at the frequency $f = 750$ THz: (a) antisymmetric mode, (b) symmetric mode and (c) isolated chain.

Figure 12 shows the dispersion of symmetric and antisymmetric transverse modes for $l = 50$ nm. Here, for the same distance as in figures 2 and 7, the coupling perturbs the propagation properties even less than the isolated chains.

Also in this case, symmetric modes allow slightly longer propagation lengths near the light line, where the coupling is stronger. Increasing the coupling ($l = 30$ nm), as in figure 13, the perturbation is stronger even if the trend is similar to that in the previous scenario. Similar to the quasi-transverse propagation considered in the previous section, these purely transverse modes are also backward in nature and support leaky-wave propagation in the upper frequency regime and the Bragg stop band in the lower one. Moreover, in this case the antisymmetric transverse mode (consistent with the definition in figure 8) supports two distinct branches, one of them with very weakly guided properties near the light line.

Figure 14 shows the calculated orthogonal electric field distribution in the $xy$-plane for the modes of figure 12 at the frequency $f = 750$ THz. In this case, the modes are purely transversely polarized and the guided wavenumbers are, respectively, $\tilde{\beta}_{\text{asym}} = 1.987 - 0.42i$, $\tilde{\beta}_{\text{sym}} = 2.64 - 0.296i$ and $\tilde{\beta}_{\text{single}} = 2.36 - 0.34i$, consistent with figure 13. The field confinement in this polarization is not drastically different from that of an isolated chain, as is evident from the figure, and the main advantage of using parallel chains may reside in the longer propagation distance of symmetric modes near the light line.
4. Conclusions

We have presented here a fully general and complete theoretical formulation for the analysis of the dynamic coupling between two parallel linear chains of plasmonic nanoparticles operating as optical waveguides. These chains may support up to eight different guided modes with different polarization properties in the same range of frequencies, which we have fully analyzed here. We have shown that, compared to linear arrays, these waveguides may support relatively longer propagation lengths and ultraconfined beams, operating analogously to transmission-line segments at lower frequencies. In particular, our results confirm that, by operating near the light line with antisymmetric quasi-longitudinal modes, we may achieve relatively long propagation lengths (of several wavelengths) and ultraconfined beam traveling, similar to a transmission line, in the background region sandwiched between the two antisymmetric current flows guided by the chains. It should be stressed that the designs considered here are based on ultrasmall nanospheres, with the aim of large concentration of light in a sub-wavelength region. This choice inherently produces relatively short propagation lengths, in part improved by the parallel chain configuration. Large field confinement, even at the expense of moderate propagation distances, may be appealing in a variety of applications, i.e. nonlinearity enhancement, sensing, optical switching and nanoscale interaction with light, as in optical nanocircuits [14, 15]. On the other hand, longer propagation distances may be achieved by considering larger particles or lower frequencies of operation for which metals are more conductive, as discussed for isolated chains in [10].

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