Optical properties of coupled silicon nanowires and unusual mechanical inductions

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Abstract
A recent study of the photonic coupling between metallic nanowires has revealed new degrees of freedom in the system. Unexpected spin torques were induced on dimers when illuminated with linearly polarized plane waves. As near-field observables, the spectra of torques showed more resolved resonances than the peaks in typical far-field spectra. Here, the study is extended to silicon dimers. The optical properties of high-dielectric systems are governed by volume resonances, not by surface resonances as is the case in plasmonic arrangements. Differently from plasmonic systems, which show strong mechanical inductions only for p-polarized light, high-dielectric systems experience the action of strong forces and torques for both polarizations s and p. The asymmetry in strong near-fields is responsible for the unusual mechanics of the system. Some consequences of this may include the breaking of the action–reaction principle or the appearance of pulling forces. This numerical study is based on an exact method. The work provides ideas for the design of nanorotators and nanodetectors. It suggests a new viewpoint about optical forces: the resultant dynamics of topological variations of electromagnetic fields.

Keywords: silicon nanowires, optical torques, morphology-dependent resonances, Newton’s third law, optical forces, dimers

(Some figures may appear in colour only in the online journal)

1. Introduction

Light is known to exert forces and torques on mesoscale objects [1]. In general, the transfer of both linear and angular momentum to the object is possible if complex beams of light are used [2]. In particular, a single plane wave having linear polarization exerts only radiation pressure on a single object that pushes it in the forward direction. Furthermore, this force has resonances that can be followed from Mie expansions as dependent on the geometry and constitution of the object in question [3]. However, with two or more optically coupled objects, the interaction between them makes the scattering very complex in general [4–7]. There is no satisfactory theoretical description covering all the phenomena involved.

As a growing research area, the field of nanophotonics demands the knowledge of the exact consequences of light–matter interactions at nano- and mesoscales. The importance of this knowledge lies, for example, in the wide possibilities already demonstrated to move, trap, or guide objects of sub-wavelength size [8–11]. Thus, the correct description of the optical forces is essential for the design of photonic-based small devices [12, 13], especially in biology [14–17], optical matter [18–20], and optical circuits [21, 22], among other subfields.

In particular, dimers’ electromagnetic scattering is very well known under the so-called small particle approximation or Rayleigh regime [3]. Under this regime, the objects’ response is represented by the coupling of dipole moments induced by the incident and the scattered fields [4, 23, 24]. As a result of the coupling, binding forces appear in addition to the scattering forces or radiation pressures exerted by light [4, 25–27]. On the other hand, the forces exerted on a dimer...
can be calculated exactly by a proper integration of the Maxwell stress tensor [28]. In particular, unexpected optical torques have been found to be exerted on metallic dimers of infinite nanowires under illumination with a plane wave having linear polarization [29–31]. Surface plasmon resonances were found to induce these torques together with the usual components of the optical forces. The results have no precedent in the literature, and cannot be approached by small particle approximations.

In this paper, the study of the optically-induced mechanics is extended to dielectric nanowire dimers. In particular, silicon is chosen for the simulations as it is a very useful high-contrast dielectric [32]. A high-contrast dielectric can sustain electromagnetic modes that correspond to morphological dependent resonances (MDRs) [33–35]. These modes correspond to volume resonances whose optical properties are very different from surface resonances [36]. For example, the former resonances have strong field concentrations inside the wires’ volume, while the latter ones enhance the fields around the surface of the objects. Another difference between high-dielectric and plasmonic systems is that the former systems have both strong electric and magnetic resonances, while the plasmonic systems have only electric spots in general [37–41]. In particular, this fact corresponds to having strong resonances under both fundamental polarizations, $s$ and $p$, in two-dimensional (2D) problems with high-contrast materials [42]. The dielectric properties of silicon have been summarized in [35], for instance. An interband direct transition induces a big enhancement of the relative dielectric function with respect to the typical value $\varepsilon_r \approx 12.25$ that is taken as the quasistatic limit [43]. Then, Mie resonances can be induced by silicon objects in the optical regime. These resonances result in strongly-confined near-field regions [44, 45] and in narrow peaks in the far-field spectra as a result of the interference [46].

As no exact analytical model exists for systems of coupled dielectric wires [47], a complete numerical study is performed here of the MDRs in coupled wires of silicon. The aim of the work is to show how new degrees of freedom appear for the dielectric dimer when the realistic interaction between the wires is taken into account. Hybridized MDRs appear in the dimers’ responses with respect to the MDRs of isolated-like objects [48, 49], as occurs with plasmonic dimers which present hybridized plasmonic resonances [24, 29, 31]. A new relation between mechanical and field observables is realized. It shows how strong asymmetries of the near-field distribution induce strong force components or torques, or other interesting effects like the breaking of the action–reaction law [50] or the eventual presence of pulling forces.

Although an exact electromagnetic method is used here, neither thermal nor Brownian forces are considered [51]. Also, no ‘dynamic’ forces are calculated, i.e. forces that take into account initial velocities and accelerations of the wires [52]. Thus, no complete dynamics is obtained for the system. However, the methodology presented here is believed to approach the movement of coupled particles with more accuracy than in previous works; see for instance the dielectric dimer results in [52] or the results in [53, 54] for plasmonic systems. The spectra of the mechanical inductions can be used to design nanorotators, nanosystem filters or nanodevices [55].

The whole methodology used in this work is based on an integral formulation of the Maxwell equations that is generally known as a version of the T-matrix method [56, 57]. Specifically, the formulation was presented in previous papers with the focus on the force calculations [29, 31, 58]. However, as we are now concerned with morphological excitations, the whole methodology is revised in the appendix for the interested reader. Time-harmonic dependence of fields $\exp(-i\omega t)$ is assumed. Two coupled scatterers are considered to be parallel to each other and to have axial symmetry along the $z$-axis. The wavevector $k_0$ is transversal to the $z$-axis. Its magnitude $k_0 = 2\pi / \lambda$ is provided by the incident wavelength $\lambda$. Under this setting, two fundamental polarizations exist which can be used to express any solution of the scattering by the system. They correspond to an electric (magnetic) field aligned with the $z$-axis, namely polarization $s$ ($p$) respectively. For details about the geometrical configuration of the system, see the appendix.

2. Results

From here onwards, the forces and torques will be shown as scaled magnitudes (for details, please see the appendix). The force densities will be given in the same units as the optical cross sections in two dimensions, i.e. in units of nm. Thus, they are fully comparable to the observables of the system in the far-field region. The 2D torques, as given in nm$^2$, count as an effective 2D volume of action of the induced forces.

The system of an isolated silicon wire is studied first in order to explore the influence of the MDRs on the forces. The results are analyzed in terms of 2D Mie expansions to identify the MDRs as multipolar contributions. This part is fundamental to the understanding of the optical response induced in the dimer system given further below.

2.1. Preliminary results: isolated wires

2.1.1. Far-field properties. Figure 1 illustrates the appearance of the MDRs in realistic silicon wires and its influence on the induced forces. An evolution of modes can be seen in figure 1(a) for a silicon nanowire as a function of the radius $R$. The detailed calculations offer a general overview of the MDRs expected for the spectra of radiation pressures at one particular value of $R$. Wires with radii $R = 40, 50$ nm will be chosen throughout this work. Figures 1(b) and (c) show the spectra for the case $R = 50$ nm of figure 1(a) for each fundamental polarization respectively. Curves in black (red) line in figures 1(b) and (c) correspond to the extinction (radiation pressure) cross section. All the results of figure 1 have been calculated by the integral method. However, the MDRs have been identified with labels obtained by 2D Mie calculations up to the $l = 3$ angular orders. The curves in figure 1(a) have been shown before in [35], and the integral...
method had already been compared against Mie theory, giving very accurate results. Notice the appearance of several modes for relatively small wires at the sub-wavelength scale. This is possible due to the high values of the permittivity given by the dielectric function of silicon. The dispersion curves of the MDRs do not result in straight lines, because the permittivity is a spectral function. An empirical rule $l_p = l_s - 1$ can also be appreciated for the first modes that appear in the spectra. With the exception of the first MDR for $s$-polarization, the locations of the MDRs in the spectra are very similar for both polarizations.

Fast growth can be observed for the curve $l = 0$ of the polarization $s$ when $R$ is increased—see figure 1(a). This fact means that the mode $l_s = 0$ can be tuned up to very long wavelengths even for wires with relatively small radii. In general, this MDR is seen to have a very different behavior from the rest of the modes in near- and far-field regimes. A more detailed study about this special mode can be found, for instance, in [33].

2.1.2. Radiation pressure. The spectra of radiation pressures and the extinctions are similar in figures 1(b) and (c) [35], with the exception of relatively small wavelength shifts in the peaks of the excitations [59–61]. Besides, the silicon dielectric function has a strong imaginary part at short wavelengths [35] that influences the shifts and the relative intensities of the force peaks with respect to the far-field observable in the high-energy region [59]. The absorption process is taken into account in the balance of the linear momentum transferred to the wire. The radiation pressure cross section gives the optimal length (2D area) to exert force by light on the wire. This mechanical magnitude is affected by the MDRs induced on the structure.

For the case of $R = 50$ nm, four MDRs can be distinguished in the $s$-spectrum of figure 1(b) and three MDRs in the $p$-spectrum of figure 1(c). Although the curves contain overlapping peaks, it can be said that the same peak resolution is obtained for both the far-field magnitudes and the forces (however, scattering and absorption cross sections

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**Figure 1.** Optical properties of Si isolated nanowires and influence of the MDRs on the optical forces. (a) Dispersion curves of the modes as a function of the radius $R$ of the wire (black/red for $s/p$-polarization in the online version). (b)–(i) For the case $R = 50$ nm of (a): (b), (c) Comparison of spectra of Radiation’s pressure cross section versus extinction under $s/p$ polarized waves. The vertical lines serve to compare the spectral locations of the MDRs. (d)–(i) Maps of the near- and inner-fields at the location of the first resonances; the small excitation at $\lambda = 378$ nm is not shown. (d)–(f) Under $s$-polarization. (g)–(i) Under $p$-polarization. The saturated color scale is labeled by the reference number, which shows the field intensity in the regions in white. As a reference, the arrow on each panel indicates the direction of the incident wave.
are not shown here). This resolution of the spectral magnitudes will be compared with that for coupled systems further below. In particular, note the structure of the first MDR corresponding to the mode \( l = 0 \) in the pressure spectra under \( s \)-polarization: the excitation is very wide and strongly overlaps with the rest of the MDRs. This behavior does not occur under \( p \)-polarization, and is a common characteristic of all the spectral curves shown in this work.

As the integral method takes the force results from the near-fields, one could expect these results to be different from those obtained by equations (A32) and (A19), a method which involves the far-fields (see appendix for details). However, no difference can be appreciated between both methods. The near-fields carry information about the contributions due to the evanescent waves but these have propagation constants parallel to interfaces of the scatterer \([62]\). The circulation of such waves around the wire surface cannot account for new contributions to the radiation pressure because the resulting field inductions are highly symmetric. The anticlockwise circulation of such waves is equal to the clockwise circulation because the incident (propagating) field is homogeneous. Then, there is no difference in using the near-field or the far-field method when dealing with the force exerted by a plane wave on a single wire.

In the same way, there is no optical torque at all for a single wire because the highly symmetric scatterer is being ‘pushed’ by plane waves with linear polarization. The wire responds with fields that resolve symmetrically with respect to the direction of the illumination—see the field maps, figures 1(d)–(i), around the wire.

### 2.1.3. Near- and inner fields

All the far-field features can be related to the field distributions of the MDRs around the wire, i.e., near- and inner fields. Here, the maps in figures 1(d)–(i) illustrate the relevant field structures around the wire of \( R = 50 \) nm of figures 1(b) and (c). Figures 1(d)–(f) show the behavior of the wavefunctions for the first three MDRs that can be appreciated from the far-fields under \( s \)-polarization. Similarly, figures 1(g)–(i) show the behavior at the location of the three MDRs that can be distinguished under \( p \)-polarization. All the electromagnetic fields are determined from the transversal fields or wavefunctions and see the appendix for details. The spectral locations of the MDRs are taken from the far-field curves; the shifts that can occur between the resonances from near- to far-fields were shown to be small—see figures 1(b)–(c). The radial and angular distribution of the fields are characterized by the integral numbers given by the Mie expansion; \( n \) corresponds to the number of maxima of the field intensity along the radial direction. On the other hand, \( 2\pi \) corresponds to the number of maxima along the azimuthal angle from 0 to \( 2\pi \) rad.

Observe the structure of the fields under \( s \)-polarization, panels 1(d)–(f). Note that the wavefunction, in this case the electric field, is not confined to the wire region. The field distribution is spread to another bigger region as if it were confined to the inside of a scatterer the size of which is bigger than the real one. On the contrary, under \( p \)-polarization, figures 1(g)–(i), the wavefunction is the magnetic field and it is strongly confined into the wire region or the region where the high-contrast medium exists. Thus, in general, we will see that the \( p \)- or magnetic modes are much more confined and more enhanced than the \( s \)- or electric modes.

The near-field structures of the MDRs are seen to be well characterized by their radial and polar modulations. Although the MDRs have an intrinsic bulk nature, they can eventually induce some surface concentration of the fields, as seen in figure 1(i). This effect is a result of the interference of the scattered and the incident fields. Another result of this interference is the ‘blowing’ effect that can be seen in the patterns. The incident fields distort the near-field structures as if they were blown to the forward direction with respect to the illumination.

It is worthwhile to notice the huge enhancement of field intensity obtained for the first MDRs under \( p \)-polarization figures 1(g)–(h). This behavior will play a key role in the forces and torques induced in systems of coupled wires.

The maybe trivial behavior of the MDRs shown on the single-wire forces will not prevail for systems of coupled wires. The complex interaction between the wires will be manifest in the coupling of MDRs in dimer systems. The scheme of hybridization of MDRs is not simple, and consequently entails unusual properties in the optomechanical inductions.

### 2.2. Homodimers

The homodimer system will be explored only for illumination with its wavevector \( \mathbf{k}_0 \) perpendicular to the axis of the dimer, labeled as \( \varphi_0 = 90^\circ \) (for details about the definition of \( \varphi_0 \), please see the appendix). The other relevant illumination studied in this paper is an incident wave with its wavevector \( \mathbf{k}_0 \) parallel to the dimer axis, which is labeled as \( \varphi_0 = 0^\circ \). A more comprehensive study of the inductions for illumination with \( \varphi_0 = 0^\circ \), \( 90^\circ \) will be carried out in the section below devoted to heterodimers. The coupled wires present hybridized resonances with respect to the resonances of the isolated wires. The induced forces and torques are presented by means of a particular example for a gap of \( d = 5 \) nm between the wires.

#### 2.2.1. Far-field properties

The far- and near-field responses of the homodimer are shown in figures 2(a) and (b) and (c)–(h), respectively. Notice the behavior of the extinction cross sections when the gap is varied; the response of the single wire \( R = 50 \) nm is also shown for comparison (curve in dark yellow line in online version; see figures 2(a) and (b)). Although very different gaps have been calculated, the MDRs remain almost at the same spectral locations with the exception of the first mode of the dimer under \( s \)-polarization (the one with the lowest energy). This mode presents a great shift of the spectral location with the gap variation if compared against the position of the MDR \( n = 1, \ i = 0 \) of the single wire; see the previous results for details.

Despite the fact that there is no realistic hybridization model for dielectric wires, it is easy to speculate that the
Dimer modes can be built with multiple multipolar single-wire resonances, in a manner similar to what is found for surface resonances in metallic dimers [24]. This hybridization has been realized for silicon dimers of 3D spheres [39, 40, 48]. The photonic transitions $\Delta l = 0$ are characteristic in the series expansions of the eigenfunctions of each wire over the functions of the other wire [28]. In this way, one can argue that the modes $n_{nm} = 1, l_{sm} = 0$ of single wire for $m = 1, 2$ must be important in the hybridization of the first $s$-mode as they conserve a similar spectral structure—see figure 2(a). However, as this MDR appears widely spread in all the spectra, their excitations are not so relevant in the system’s characterization.

The rest of the MDRs remain quite static in the spectra as the gap is varied for the two polarizations. Actually, the spectrum for the homodimer is very similar to the single-wire spectrum under both polarizations. This is due to the nature of the MDRs as volume resonances. The fields at these resonances are very confined to the wires’ region and the spectral curves are not so sensitive to the geometric variations of the dimer, with the exception of the shifts in the spectral locations of the first MDR. On the other hand, there are strong variations of the intensities of the MDRs with the gap. In particular, for the shortest gap, the $s$-extinction reaches maxima almost twice those reached by the $p$-extinction—see the second peaks in figures 2(a) and (b).

2.2.2. Near- and inner fields. The maps of near- and inner fields of figures 2(c)–(h) help us to give a better idea of the hybridizations of MDRs that occur in the homodimer. For the sake of clarity, the most relevant maps are shown here; the highest-energy modes that appear at $375 - 380$ nm are not shown. Thus, four modes are shown in figures 2(c)–(f) for $s$-polarization. Similarly, two MDRs are shown in figures 2(g) and (h) for $p$-polarization.

In general, the maps show a strong coupling of the fields that resonate at each wire. However, as said, the inner structures of the MDRs can be observed to be similar to those found for the single wire. The map figure 2(c) appears to support the hypothesis of the hybridization of the modes $n_{nm} = 1, l_{sm} = 0$. Similarly, figure 2(g) shows an analogous behaviour for $p$-polarization, i.e. a hybridization of the modes $n_{nm} = 1, l_{pm} = 0$. The maps in figures 2(d) and (e) show a strong...
influence of the single-wire modes $n_m = 1$, $l_m = 1$, which open up to both sides due to the effect of the illumination and the multiple scattering. Figure 2(h) shows a similar behavior for $p$-polarization but, in this case, the structures close up to the inner region between the wires. Again, a big field concentration is obtained under $p$-polarization. Notice the values of the intensity reached in figures 2(g) and 2(h) which are several times the value given by the incident wave.

2.2.3. Homodimers’ forces. The methodology for calculating the mechanical magnitudes is the same as that presented in [29, 31]. The resultant curves use the same color code as the circles of integrations (see inset schemes); black for the wire (1) on the left which is enclosed by $C_1$, red for the wire (2) on the right which is enclosed by $C_2$ and green for the whole system which is enclosed by $C_3$. It is worthwhile to clarify that the curve $C_3$ can be arbitrary as long as it properly encloses the entire system; it could be a circle as well as any other circles of integrations $[C_i]$. The resultant curves use the same color code as the mechanical observables—see also figure 3(c). Even the highest-energy mode can be seen to appear lightly in the forces around $\lambda \approx 375 - 382$ nm.

Under the configuration $\phi_0 = 90^\circ$, the force components of scattering and binding can be distinguished—see figures 3(a) and 3(b); curves in dotted black and solid green are scattering components while those in solid black and red are binding components. Both sets of curves carry the information of the interaction between the wires. Of course, the system is pushed ‘down’ as a whole in the $-y$ direction by radiation pressure due to the incident waves (green curves in figures 3(a) and 3(b)). The black dotted curve represents two equal contributions for the induced density of force along the $y$-axis, each corresponding to one wire. This curve is logically half of the green curve for the induced force for the system, i.e. $dF_y(C_2) = dF_y(C_1) + dF_y(C_2) = 2dF_y(C_1) = 2dF_y(C_2)$.

To estimate the effect of the coupling on the radiation pressure, one can compare the curves of the scaled $y$-forces of figures 3(a) and (b) with the scaled force for single wire as $\frac{1}{4\pi\epsilon_0}|E|^2$, obtained by equation (A32), where $C_{pr}$ is given in figures 1(b) and (c). The $y$-forces have the same order of magnitude than the radiation pressure for the single wire.

It is worthy of note that the binding forces show an attractive behavior under both polarizations in all the

![Figure 3](image-url)
2.2.4. Homodimers’ torques. As was found in metallic dimers [29, 31], unexpected torques are induced by linear polarization as a result of the realistic interaction between the silicon wires—see figure 3(c). In this case, due to the nature of the MDRs, the spin torques are obtained under illumination with both polarizations s and p—see dotted versus solid curves respectively in figure 3(c). Although no net induced torque exists for the system, net spin torques exist for each wire and they appear in coördinated form [29]. Observe that the red and black curves in figure 3(c) are always equal but opposite in such a way that they are always balanced to zero for the whole system. This is expecte due to the homodimer’s symmetry.

In addition, as was expressed previously [29, 31], the spectral spins have in general more resolution than the optical forces. The peaks corresponding to the MDRs are narrower and less overlapped than those found in the spectra of forces. This conclusion is now of general validity in a way independent of the materials of the wires, and this will also be concluded for the heterodimers’ case. The torques are suitable observables of the system and they are also preferable when choosing a near-field observable of the wires’ interaction. Even more, the torques carry information about the interaction that is not included in the induced forces. The signs of the spin torques at the spectral locations of the MDRs constitute one example of this. While the induced binding forces have the same sign in all the spectra s, p, the torques do not. In this way, the definition of bonding and antibonding of the modes needs to be revised, as was pointed out in [31] for metallic dimers.

In the spirit of the previous works, a new relation can be realized between observables of both near- and far-fields. With this hypothesis at hand, the maps of figure 2 can be examined to give an explanation for the torques found in silicon dimers. Remarkably, there is a connection between the torques and the presented maps because there is no induced torque for the first MDRs under both s- and p-polarizations—see figure 3(c). The first MDR is expected for s-polarization at $\lambda \approx 1395-1400$ nm—see figure 2(c)—and there is no induced torque for long wavelengths in figure 3(c). Similarly, the same occurs under p-polarization; the first MDR is expected to appear around $\lambda \approx 545$ nm but this resonance does not appear in the spectra of the induced torques—see figures 2(g) and 3(c) with its inset graphic. The reason for this feature is that the two near-field patterns at these locations are highly symmetric, while the other maps clearly show symmetric but bent orientations. These stationary orientations have specular symmetry with respect to the y-axis or the illumination direction but show a preferable angle—see figures 2(d)-(f) and (h). These asymmetries support a reason for the spin torques to exist in silicon homodimers. Some kind of symmetry breaking is induced by the photonic interaction itself, and this would produce the spins. Meanwhile, the gradient of the field distributions in the gap between the wires seems to play a role in bringing the wires together.

A geometric symmetry breaking exists for heterodimers because the wires are dissimilar. Thus, an asymmetric-field induction will appear that originates spin as well as orbital torques. These effects are explored in the following section.

2.3. Heterodimers

In this section, an example of parameters $r_1 = 50$ nm, $r_2 = 40$ nm and $d = 5$ nm is taken as an illustration of the unusual properties of silicon heterodimers. The MDRs can be altered due to geometric variations, relative changes in the angle of the incident wave or polarization shifts. Here, a study is realized for the two relevant directions $\varphi_0 = 0^\circ, 90^\circ$. The reason for including the configuration $\varphi_0 = 0^\circ$ will be clear when the mechanical results are analyzed. As above, the results in far- and near-fields will be related to the mechanical results.
2.3.1. Far-field properties. The far-field responses at \( \varphi_0 = 0^\circ, 90^\circ \) are compared between themselves for both polarizations \( s \) and \( p \) in figure 4. The spectra for the isolated wires have been also added for comparison, i.e. the cases \( R = 50 \) nm and \( R = 40 \) nm. The differences between the heterodimer spectra and isolated-wire spectra already indicate a possible hybridization scheme for the MDRs of the system. The coupling between the wires changes the energies of the MDRs of the heterodimer. The vertical lines drawn in the figures help to establish possible relations between the MDRs of the different spectra.

The first MDR for the heterodimer under \( s \)-polarization is shown to be very sensitive to the coupling if compared with the first MDRs of the isolated-wire curves. In contrast, poor sensitivity is found for the MDRs of the system under \( p \)-polarization; the MDRs seem to have almost the same spectral locations as the MDRs for the isolated wires. For the two fundamental polarizations, both spectra \( \varphi_0 = 0^\circ, 90^\circ \) show almost the same spectral location for the first MDR.

On the other hand, the extinction under illumination with \( s \) with \( \varphi_0 = 0^\circ \) is recognized for a strong excitation at \( \lambda = 790 \) nm—see figure 4(a). In practice, this MDR can be excited by means of an illumination with a Ti:sapphire laser tuned to this wavelength [63]. There is no other MDR in this spectral region for illumination with \( \varphi_0 = 90^\circ \).

The heterodimer peaks that appear at locations similar to the isolated-wire peaks for the curve \( R = 40 \) nm are characteristic of the heterodimer. In other words, those MDRs in high-energy regions allow us to identify the dissimilar wires by means of the intensity of the spectra under \( p \)-illumination with \( \varphi_0 = 90^\circ \). Note the peaks’ intensities at \( \lambda \approx 400; 470 \) nm in the red curve of figure 4(b).

For one particular polarization, almost all the MDRs lie in the close spectral locations between them. There is one special exception for the \( s \)-peaks at \( \lambda \approx 525; 565 \) nm, see curve in red line in figure 4(a). They seem to be a splitting of the \( \lambda = 550 \) nm peak of the isolated-wire curve \( R = 50 \) nm (in dark yellow line). This may be a result of the hybridization scheme for this particular example of silicon heterodimers. On the other hand, all the curves shown have very different intensities of excitation of the MDRs from those in the spectra of isolated wires. This phenomenon is another consequence of the coupling of the wires, and could be properly described by an adequate hybridization model.

2.3.2. Near-field properties. To gain knowledge about the coupling between the wires and its behavior in the far-field region, the relevant near-field maps are shown. These maps illustrate the spectral locations of the first MDRs (lowest-energy modes)—see figures 5–8. The maps of figures 5 and 6 correspond to the angles \( \varphi_0 = 0^\circ, 90^\circ \) respectively for polarization \( s \), while the maps of figures 7 and 8 correspond to \( \varphi_0 = 0^\circ, 90^\circ \), respectively, for polarization \( p \).

In general, it is easy to see how several hybridized MDRs enter into the spectra when the energy is growing—see figure 4. The maps for heterodimers clearly show the symmetry breaking in the structure by means of asymmetric-field patterns. Logically, the patterns under the configuration \( \varphi_0 = 0^\circ \) hold the symmetry with respect to the \( x \)-axis while the patterns under illumination with \( \varphi_0 = 90^\circ \) do not hold any symmetry, i.e. symmetry is broken with respect to both the \( x \) - and \( y \)-axes.

The monopolar modes for the whole structure appear in figure 5(a) and in figure 6(a) for polarization \( s \) in a way analogous to the mode found in figure 2(c) for \( \varphi_0 = 90^\circ \). Let us call it monopolar mode, in analogy with the single-wire mode \( n_s = 1, l_s = 0 \); this definition is also used in the nomenclature of the molecular theory [64]. In particular, the maximum field distribution occurs around wire 1 for figure 5(a) as if the illumination would blow the scattered field to the left. In addition, the effective wavelength \( \lambda_{\text{eff}} = \lambda/\sqrt{\text{eff Si}} \) at this energy is too long to include a modal structure inside wire 2. On the other hand, the patterns of the maps of figures 2(c) and 6(a) are very similar, but this latter one resolves asymmetrically with respect to the \( y \)-axis due to the geometric symmetry breaking of the dimer.

The strongest MDR that appears in figure 4(a) at \( \lambda = 790 \) nm under illumination \( s, \varphi_0 = 0^\circ \), corresponds to the field pattern of figure 5(b). Interestingly, the scaled field intensity reaches around nine times the intensity of the incident field. This map structure of the fields seems not allowed to exist for polarization \( s \) and \( \varphi_0 = 90^\circ \)—see maps of figure 2 for homodimers’ resonances and figure 6 for heterodimer’s resonances. It is a characteristic mode of the configuration \( \varphi_0 = 0^\circ \). The pattern resembles a mode like \( n_s = 1, l_s = 1 \) for isolated wire as if it were the response by a bigger wire corresponding to the entire system. However, the structure could also be seen as the hybridization of two monopolar modes of isolated wires. The rules of hybridization are not applicable with realistic wires.

The next two patterns in figures 5(c) and (d) resemble hybridizations using the first single-wire MDRs. Pattern 5(c) appears to be built with combinations like \( n_{sr} = 1, l_{sr} = 1 \) and 5(d) like \( n_{ls} = 1, l_{ls} = 1 \) with \( n_{ls} = 1, l_{ls} = 0 \). Figures 5(e) and (f) could show molecular-like hybridizations of \( n_s = 1, l_s = 2 \) with \( n_s = 1, l_s = 1 \) and with \( n_{ls} = 1, l_{ls} = 0 \), respectively. These cases would give non-trivial rules of energy orders for the multipolar modes of the entire structure.

Following the analysis of the maps of figure 6, the patterns also begin to hybridize low-order modes and they start including patterns corresponding to single-wire MDRs of higher orders when \( \lambda_{\text{eff}} \rightarrow 0 \). The maps of figures 6(d) and (e) show complex field conformations and modulations around and inside of the high-contrast material of the wires. The intensity spots show multiple connections with each other. In particular, strong field enhancements are obtained thanks to the presence of a dipolar-like mode in the biggest wire—see figures 6(b) and (c).

On the other hand, figures 6(b) and (c) are closely related to the peaks found in the curve in red line of figure 4(a). It was expressed that those peaks seem to be a splitting from the single-wire MDR \( n_s = 1, l_s = 1 \) for \( R = 50 \) nm. This mode is seen to play a key role in the maps of figures 6(b) and (c), as it is the main excitation in the hybridized mode.
The analysis of the near-field structures under \( p \)-polarization becomes more interesting. The intensities of the magnetic field reach enormous values with respect to the intensity of the illumination—see the referenced values of the saturated scales in the panels. But even more interesting is the fact that the field enhancements can be tuned to one wire or the other by choosing the proper incident wavelength—see, for instance, figures 7(a) and (b), or (c) and (d). Of course, the patterns are not symmetric, as said, for heterodimers and they go on to include higher-order modes for higher energies; but the ‘alternacy’ of the enhancement locations on the inner fields can also be seen when comparing figures 8(a) and (b), or (c) and (d). This alternacy will be seen to have a connection with the dynamics of the dimer because it ‘plays’ with the ‘optical inertia’ induced on the wires.

Another remarkable effect occurring in the silicon dimers comprises the strong electric fields that can be obtained for the design of applications due to the presence of...
For instance, the intensity of the electric field around the gap region is around six times the value of the incident wave—see figure 2(d). Similarly, strong magnetic fields can also be obtained as in figure 7(b). Although high-dielectric wires produce volume resonances that confine the fields inside the wires, the enhancements are so big that they compete with those obtained by plasmonic structures or systems that can have surface resonances [36]. Even more, the coupled wires of silicon provide great intensities for both electric and magnetic fields, or for the two fundamental polarizations, which is not the usual case with 2D plasmonic structures [65].

Figure 7. Near-field maps of the modes of the Si heterodimer of radii $r_1 = 50$ nm, $r_2 = 40$ nm and $d = 5$ nm under $p$-polarization. The incident angle is $\varphi_0 = 0^\circ$. The saturated color scale is labeled by reference numbers which show the field intensity in some regions in white.

Figure 8. Near-field maps of the modes of the Si heterodimer of radii $r_1 = 50$ nm, $r_2 = 40$ nm and $d = 5$ nm under $p$-polarization. The incident angle is $\varphi_0 = 90^\circ$. The saturated color scale is labeled by reference numbers which show the field intensity in some regions in white.
2.3.3. Heterodimers’ forces under illumination with $\phi_0 = 0^\circ$.

The mechanical response induced on the heterodimer by the configuration $\phi_0 = 0^\circ$ is shown in figure 9 for the polarizations $s$ (a) and $p$ (b). As the illumination saves the symmetry of the system, the induced forces are always along the $x$-axis and, of course, the induced net torques are identically zero. The illumination reaches the system by the right and the smallest wire, 2, feel an advanced pressure while each wire is simultaneously repelled from the antibonding mode, as shown by the inset scheme in figure 9 for the $s$ polarization. The red curve of figure 9 (a) is considered, since the pattern resembles the electronic distribution of an antibonding molecular mode [64]. A hot spot of the field distribution is reached in the gap region. The signs of the curves at this point in common, which means they share a common force configuration. As the illumination saves the first MDR for this configuration, the stopped wire is that labeled as 1. This is why the net densities of forces are different for each wire. Binding forces are overlapped with scattering forces for this configuration. However, a net scattering force is distinguished by the methodology of calculation for the whole system—see green curves in figures 9(a) and (b). The information of the interaction given by these force components is very interesting, and complements the studies that were done in near- and far-fields. For instance, the first MDRs for polarization $s$ do not correspond to any bonding or antibonding mode—observe figure 9(a) around $\lambda \approx 1285$ nm. The corresponding map is given in figure 5(a). Observe that the red and black curves in figure 9(a) have a crossing point in common, which means they share a common force value. Thus, the wires would be accelerated in the forward direction with respect to the illumination without attraction/repulsion between them. Simultaneously, the system also moves in the forward direction due to radiation pressure; the minimum of the green curve occurs for $\lambda = 1285$ nm.

The next mode, well ‘detected’ by the forces, corresponds to the strong MDR occurring at $\lambda = 790$ nm—see figures 5(b) and 4(a). The sign of the curves at this wavelength indicates that the MDR give place to an antibonding mode, as shown by the inset scheme in figure 9(a). Thus, the system moves as pushed by radiation pressure while each wire is simultaneously repelled from the other at this energy. The result seems quite natural when map (b) of figure 5 is considered, since the pattern resembles the electronic distribution of an antibonding molecular mode in diatomic molecules [64].

The next MDR for this configuration, located at $\lambda = 555$ nm in the curves of figure 9(a), is also related with its corresponding near-field map, figure 5(c). This map shows a bonding mode; it also resembles the electronic distribution of a bonding molecular mode [64]. A hot spot of the field distribution is reached in the gap region. The signs of the curves of forces—see black and red curves in the online version—indicate the bonding nature of this MDR in the spectra of figure 9(a).

The next MDRs enter into the spectra of induced forces as the energy grows but with decreasing absolute values. Attractive or repulsive modes enter in the spectra as the sign of the coordinated forces changes. This is a characteristic of the mechanical observables; they represent more information about the resonances than the peaks in far-field curves because the sign of the forces provides information about the modes.

The results of forces for polarization $p$ bring about more curious effects. Note that the first two MDRs, located at low energies, present an unusual force behavior in figure 9(b). If one considers some shifts between the spectral locations of the MDRs of the far-fields and of the forces, one of the wires experiences almost zero force when the other experiences the maximum value of exerted force at resonance. For the first MDR, the stopped wire is that labeled as 2 while for the second MDR, the stopped wire is that labeled as 1. This manifestation is coherent with the first two ‘alternating’ modes of figures 7(a) and (b), respectively. Although there exist some shifts in the resonant locations of these modes, the relation between near-field maps, forces and far-field curves is coherent. Observe that the net force is around zero on one wire when the inner-field concentration is minimum on this wire—see figures 7(a) and (b). The maximum field concentration for these MDRs produces the affected wire to be accelerated although the coupled neighbor is almost stopped. Of course, the force for the whole system is almost the force exerted on the wire with the focused field. Thus, the force effect of the first MDR for $\phi_0 = 0^\circ$ is as though wire 1 were pulling wire 2—figure 7(a)—while in the situation of figure 7(b), it seems like wire 2 would have to push wire 1.

When the energy is increased around $\lambda \approx 430–438$ nm, the following MDR produces a resonant positive peak in the red curve of figure 9(b) and a negative peak or resonant dip in the black curve. A repulsion state appears—namely, an antibonding mode. This repulsion corresponds to the situation...
of the map in figure 7(c). The following MDR is located at \( \lambda = 418-422 \text{ nm} \) in the spectra of forces and it has no direct relation to any map of figure 7. This results quite naturally, since more resolution of peaks is expected for forces' spectra than spectra obtained via far-fields. The overlap that occurs in far-field curves may hide this excitation for this energy region. The next MDR occurs in the forces at \( \lambda = 395 \text{ nm} \)—see figure 9(b)—and it has direct correspondence with the map of figure 7(d). The difference in the absolute value of the excitations at \( \lambda \approx 430-438 \text{ nm} \) and \( \lambda = 418-422 \text{ nm} \) indicates 'relative' attraction states between the wires—figure 9(b). The next resonance in figure 9(b) is a higher-energy mode which also plays a role in the mechanical magnitudes.

2.3.4. Heterodimers' forces under illumination \( \varphi_0 = 90^\circ \) and \( s \)-polarization. The results of the induced forces under configuration \( \varphi_0 = 90^\circ \) are provided in figure 10. Figures 10(a) and (b) show the binding forces and the scattering components for polarization \( s \), respectively. Figures 10(c) and (d) show the same for \( p \)-polarization. The configuration \( \varphi_0 = 90^\circ \) is the most relevant of the present study as more induced torques appear in the symmetry-broken system than in homodimers—see figure 11. Note that all the induced peaks of forces are comparable in order under polarization \( s \), differently from the inductions seen in figure 9(a) where a peak is relatively much stronger than the rest. In general, the induced forces for \( \varphi_0 = 90^\circ \) show more unusual properties than the previous configurations—in particular, see the resonant spectral locations in figure 10. The validity of the action-reaction law can be evaluated for the binding forces under this symmetric illumination, as it was analyzed for plasmonic systems in [31].

The first MDR for polarization \( s \) is 'felt' by the binding forces at around \( \lambda = 1390 \text{ nm} \), compare against the far-field resonant location that is \( \lambda = 1280 \text{ nm} \), see figure 4(a). Red-shifts are expected for near-field resonances with respect to the far-field peaks [60, 61]. For the first MDR, the curves in black line and in red line are almost equal but opposite, giving zero contribution to the \( x \)-force for the system. In other words, the bound system follows action–reaction for this energy while it is being pushed down by radiation pressure—see figure 10(b) at this wavelength. From the point of view of binding forces, the first mode of the system preserves the symmetry although the natural symmetry is broken—see figure 6(a). In other words, the system does not feel any lateral force for this mode.

The second mode that appears in the spectra of figure 10(a) is given around \( \lambda = 780-800 \text{ nm} \), depending on which curve is analyzed. If compared against the previous results, one may conclude that this mode corresponds only to the configuration \( \varphi_0 = 0^\circ \)—see figures 5(b) and 9(a). As found in previous works for plasmonic systems, the forces have enough resolution to 'detect' peaks of excitations of \( \varphi_0 = 0^\circ \) under an illumination with \( \varphi_0 = 90^\circ \). This phenomenon is a consequence of the evanescent waves present in the multiple scattering between the wires. The evanescent waves save information of the interaction regardless of the specific conditions of the illumination [66]. Furthermore, under this excitation there exists a breaking in the action-reaction principle which gives place to a net lateral force for the whole system, see the green curve in figure 10(a) around
The incident angle is $\lambda = 800$ nm. The general situation of the resultant binding forces is given by the inset scheme in figure 10(a) for this particular resonance. On the other hand, the radiation pressure or scattering force may not appear as resonant for this wavelength, see figure 10(b). This is probably due to the fact that the overlapping effects mask the corresponding excitation.

From figure 10(a), a third MDR can be seen to appear at $\lambda = 572$ nm. In the far-field, this MDR is seen at $\lambda = 565$ nm, figure 4(a). For this mode, there is no resultant $x$-force for the whole dimer (green curve in figure 10(a)). This mode preserves the action–reaction law. The resonance corresponds to the pattern shown in figure 6(b) in order to establish a relation with the near-field. However, the relation of this MDR with its corresponding scattering force results difficult, because the closest realistic excitation appears in figure 10(b) at $\lambda = 530–555$ nm depending on which curve is observed ($\lambda = 530$ nm for the green curve). That is, the fourth and fifth MDRs can be distinguished to appear at $\lambda = 532–538$ nm and $\lambda = 472–484$ nm respectively in figure 10(a). Following the maps of near-fields, the closest resonances that were obtained from far-fields occur at $\lambda = 525$ nm and $\lambda = 475$ nm—figures 6(c) and (d), respectively. The overlap and the shifts of the excitations make the desired relation difficult to apply between the curves in black, red and green of the two panels (a-b) of figure 10. However, a very interesting result is obtained in figure 10(b) for the MDR around $\lambda = 555$ nm. An almost vanishing pulling force is obtained on wire 2 under plane-wave illumination and polarization $s$—see inset scheme on the panel for graphical clarification of the effect. Logically, this behavior will lead us to relatively strong orbital torques—see below in figure 11 and its subsequent analysis.

The bonding property of the first three MDRs can also be noted by the sign of the curves at resonances in figure 10(a). The fourth distinguishable MDR in figure 10(a) changes the signs of the curves, and it gives an antibonding mode at $\lambda = 530$ nm. The abrupt transition between the third and the fourth MDRs in figure 10(a) can be understood by comparing the maps from figures 6(b) and (c). In the former map, figure 6(b), the system seems bound by the field structure, while in the latter map, the antibonding ligation can be linked to the appearance of the isolated spot inside wire 2. Note the absence of the field around this spot in contrast to the field penetration inside the same wire in figure 6(b). In addition, at this fourth resonance, the system has also a net lateral force which resolves as negative—see the green curve at $\lambda = 538$ nm. Thus, another breaking of action–reaction appears and the dimer would now be accelerated back in the $-x$ direction.

At higher energies, the binding forces include more MDRs in figures 10(a) and (b) before the appearance of the highest-energy excitation, located around $\lambda = 370–385$ nm. The relation between the curves is complex again because of the overlapping peaks and the shifts between the excitations of the different curves. However, another remarkable effect is the successive excitations that are manifested in the green curve for the whole system. Each MDR that is excited originates a breaking in the action-reaction law and pushes the dimer along $x$ or $-x$ direction while it is being pushed also by radiation pressure along $-y$ direction. This is an interesting phenomenon because it would allow distinguishing...
homodimers from heterodimers in a hypothetical experiment
with mixed systems. The deviation from the forward
trajectories with respect to the incident direction \( \varphi_0 = 90^\circ \)
would be a signal of the present heterodimers—see figure 3
for a comparison with homodimer’s induced forces.

### 2.3.6. Heterodimers’ torques

As anticipated, the induced torques correspond to the previous results of forces and fields
of the heterodimer—figure 11. Figures 11(a) and (b) show the results under polarization \( s \) and \( p \) respectively. Here, the
curves in black and red represent spin torques induced on
wires 1 and 2, respectively, and the curves in green, which are
not identically zero, represent orbital torques for the entire
dimer. A particular situation at \( \lambda = 550 \) nm is represented
with the inset scheme on figure 11(a). The green scale at right
in figure 11(a) corresponds to the values obtained for the
curve in green which reaches approximately one order of
magnitude more than the values for spin torques (left ordinate
scale). As a complement, figure 11(c) illustrates the behavior
of the unusual spin torque induced on wire 1 as a function of
the gap between the wires. These torques are induced at the
He—Ne laser wavelength of \( \lambda = 632.8 \) nm, and two curves
are shown for each fundamental polarization. The vertical
scale on the left (right), in black (red) color, corresponds to
the induced torques for polarization \( s \) (\( p \)).

First, note in figure 11(a) that the ‘monopolar’ MDR is
now allowed to appear in the spectra of torques. Compare
the situation against the similar homodimer configuration in
figure 3(c), where only spin torques exist. Furthermore, the
structure of the curve in green line in figure 11(a) seems to
indicate that there is some overlap of excitations at low
energies (long wavelengths). The curve in green for
polarization \( s \)—see figure 11(a)—appears to have an overlap
between the peaks at \( \lambda \approx 1280 \) nm and \( \lambda \approx 780–890 \) nm.
Remember that the MDR at \( \lambda \approx 780–890 \) nm appears in the
far-fields for \( \varphi_0 = 0^\circ \) as a consequence of the interaction.
Moreover, these peaks appear as resonant spin torques but
with vanishing values in the curves in black and red of
figure 11(a) (zoom details not shown here).

Due to the high resolution that the torques offer as near-
field magnitudes, several narrow resonances enter the scene
for both polarizations as the energies grow—see figures 11(a)
and (b). Although these peaks are relatively narrow and very
resolved, they appear as one after the other. Taking also into
account the shifts between the different curves of integration,
the relations between the MDRs of these curves are difficult
to deal with. However, several MDRs can be recognized
because they are supposed to appear in the far- and near-fields
at close spectral locations between them. The remarks to be
made in the analysis of figure 11(a) are as follows. (1) Strong
orbital and spin torques are induced at the interval \( \lambda \in
(522–565) \) nm and at \( \lambda \leq 474; 420 \) nm for polarization \( s \). (2)
These inductions correspond to the resonances with strong
asymmetric fields that show the maps in figures 6(b) and (c)
in the former case. (3) The MDR found at \( \lambda \approx 474 \) nm is
related to the map in figure 6(d).

For polarization \( p \), figure 11(b), the MDRs are clearly
identifiable in the torques at \( \lambda = 635 530 430 400 \) nm. The
MDRs located at \( \lambda = 430, 400 \) nm are related with the field
distributions of figures 8(c) and (d). The strongest induction
occurs at \( \lambda = 530 \) nm (big peak in the curve in green for
orbital torque) and it would correspond to the MDR in
that include multiple scattering. Some of the effects of unusual inductions can only be seen with realistic calculations under plane-wave illumination with linear polarization. The coupled wires made of high-dielectric materials. In particular, in this work, new mechanical effects have been explored on more unstable.

The pulling force shown in figure 10(b) is obtained exactly at the same wavelength.

Finally, a variation of the spin torque with the gap will be discussed as another illustration of the new optical effects presented here—figure 11(c). The range of gaps goes from the studied value \( d = 5 \, \text{nm} \) up to \( d = 1600 \, \text{nm} \). Notice that the laser wavelength is very near to the minimum found for the orbital torque (curve in green line) at \( \lambda = 635 \, \text{nm} \) for polarization \( p \) in figure 11(b)—see in particular the inset graphic. This results in an absolute minimum for the \( p \)-spin torque at \( d = 5 \, \text{nm} \)—see curve in red in figure 11(c). Surprisingly, the spin presents damped oscillating behavior with the gap around the zero value (blue line) for both polarizations. In particular, the maximum spin is not reached at \( d = 5 \, \text{nm} \) under illumination with polarization \( s \)—see the curve in black. The absolute maximum reached for polarization \( s \) occurs at \( d = 185 \, \text{nm} \) for this example. Furthermore, the curve in black has several extremals and several zeros (compare against the blue line) at specific values. Both curves present zero torque when \( d \rightarrow \infty \) as the physical limit of isolated wires is reached. On the other hand, the curves \( s \) and \( p \) show a different behavior at the near-field distances.

Regarding the spin torques, there is an interesting remark when the results for high-dielectric dimers and metallic dimers are compared (results for metallic dimers not shown here). For metallic dimers, the spin torques decay rapidly in absolute value with the increasing gap. The response is quite different in the example shown for silicon heterodimers, as the spin state holds for gap distances equivalent to many characteristic wavelengths for polarization \( s \).

This essential difference in the mechanical responses is due to the nature of the resonances excited in each case. For the case of metallic systems, the resonances obtained correspond to surface modes. For the case of dimers made with high-contrast dielectrics, the resonances excited correspond to volume modes. The field concentration for the latter modes lies mainly inside the particles. However, the near-fields spread out for polarization \( s \). Thus, the spin torques can be sustained along great distances. Nonetheless, the configuration \( \varphi_0 = 90^\circ \) is unstable in all the spectra of dimers. The system will try to align itself with the illumination direction. In particular, for homodimers, the contributions of orbital torques arise as soon as the configuration \( \varphi_0 = 90^\circ \) is left. For heterodimers, the contribution of the orbital torques always exists for incident angles \( \varphi_0 \neq 0^\circ, 90^\circ \), so the system is even more unstable.

3. Conclusions

In this work, new mechanical effects have been explored on coupled wires made of high-dielectric materials. In particular, the results were illustrated on two-dimensional silicon dimers under plane-wave illumination with linear polarization. The unusual inductions can only be seen with realistic calculations that include multiple scattering. Some of the effects of including multipolar radiation may involve pulling forces, broken action—reaction law, lateral forces for the entire dimer or spin and orbital torques in addition to the well-known binding and scattering forces.

The mechanical inductions have been related to the MDRs that can be excited in systems with a high-dielectric material. The study has included the response of single wires as a way to introduce MDRs and their complex mechanical inductions when the wires are coupled. In particular, strong anisotropic fields are obtained in heterodimer systems due to the excitation of MDRs that induce strong torque components in the structure.

The spin torques at illumination configurations with \( \varphi_0 = 0^\circ, 180^\circ \) are unstable because orbital torques also exist for the system (only the cases \( \varphi_0 = 0^\circ, 90^\circ \) have been shown here). These orbital torques would cause the system to rotate towards an alignment with the illumination. As a consequence, the system may have oscillating rotation around the illumination direction while it is being pushed by radiation pressure; and it also may be accelerating in lateral directions if it has dissimilar particles, as in the heterodimer illustrated here. In the particular case of alignment with the illumination, i.e. \( \varphi_0 = 0^\circ, 180^\circ \), all the torques cease.

In particular, the unusual spin torques observed in the coupled wires constitute a new approach to the movement of the system. They should be taken into account for the design of such photonics-based nanodevices as, for instance, filters of nanoparticle systems or a ‘nanofactory’ [5]. The exhaustive study presented in this paper contributes to the completion of previous studies about the mechanical response of nanosystems [29, 31, 58, 62].

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Appendix A. Methodology

In this section, the methodology used in this work is described for the two fundamental polarizations existing in 2D scattering problems.

A.1. Integral method to obtain the exact fields

A well-known integral method is the general exact formulation used here to calculate both the near and far-fields of the dimer’s scattering [58, 67–69]. Time-harmonic dependence of fields \( \exp(-i\omega t) \) is assumed. Let us suppose two coupled scatterers having axial symmetry along the \( z \)-axis. Under this setting, two fundamental polarizations exist which can be used to express any solution of the scattering by the system. They correspond to an electric (magnetic) field aligned with the \( z \)-axis, namely polarization \( s \) (\( p \)) respectively. Then, the solution for each component of the electromagnetic field is split into two families. Each family depends on a unique
scalar function $\psi_\alpha(r)$, where $\alpha = s, p$ is the corresponding polarization. This function is the union of three piecewise solutions $\psi_j^{(\alpha)}$ on each domain $j = 0, 1, 2$ of the dimer, respectively (see figure 12). They obey equations

$$\nabla^2 - k_0^2 \psi_j^{(\alpha)}(r) = 0,$$

(A1)

$$\psi_j^{(\alpha)}(r)|_{r \to c^{i}_\alpha} = \psi_j^{(k)}(r)|_{r \to c^{i}_\alpha},$$

(A2)

$$\frac{1}{\nu_j(\alpha)} \frac{\partial \psi_j^{(\alpha)}(r)}{\partial n}|_{r \to c^{i}_\alpha} = \frac{1}{\nu_k(\alpha)} \frac{\partial \psi_j^{(k)}(r)}{\partial n}|_{r \to c^{i}_\alpha},$$

(A3)

where $j, k$ represent two continuous and adjacent media with respect to the contour $C_m$ of the scatterer $m = 1, 2$. Here, $\nabla_2$ is the transversal nabla operator and the vectors $r, k_0$ also belong to the 2D space $(x, y)$. The wavevector $k_0$ with magnitude $k_0 = \frac{2\pi}{\lambda} \sqrt{\varepsilon_0\mu_0}$—see figure (12)—is provided by the incident wavelength $\lambda$, the surrounding medium characterized by $\varepsilon_0, \mu_0$ and the incident angle $\varphi_0$. $\nu_j(\alpha)$ is a polarization-dependent factor defined as $\nu_j(\alpha) = \mu_j$ and $\nu_j(p) = \varepsilon_j$. Thus, the fields in every point in space can be obtained via the ‘principal’ field $\psi_j^{(\alpha)}$ and its complementary field $i \int_{\alpha} \nabla_2 \times \psi_j^{(\alpha)}(\mathbf{r}) \cdot \hat{\mathbf{z}}$, where $\nu_j(\alpha)$ is another polarization-dependent factor defined as $\nu_j(\delta) = \mu_0$ and $\nu_j(p) = \varepsilon_0$. For the sake of clarity, they are specified below for each polarization:

$$E^{(s)}(r) = \psi_j^{(s)}(r) \hat{\mathbf{z}},$$

(A4)

$$H^{(s)}(r) = \frac{i}{\omega\mu_j \mu_0} \nabla_2 \times \psi_j^{(s)}(r) \hat{\mathbf{z}},$$

(A5)

for $s$-polarization, and

$$E^{(p)}(r) = \psi_j^{(p)}(r) \hat{\mathbf{z}},$$

(A6)

$$H^{(p)}(r) = \frac{i}{\omega\varepsilon_j \varepsilon_0} \nabla_2 \times \psi_j^{(p)}(r) \hat{\mathbf{z}},$$

(A7)

for $p$-polarization.

With the convention of normals as shown in figure 12, the expressions for the scattered field on each medium $j = 0, 1, 2$ can be written as

$$\psi_j^{(0)}(r) = \psi_j^{inc}(r)$$

$$+ \frac{1}{4\pi} \int_{c^1} ds' \left[ G_0(r, r') \psi_j^{(0)}(r') - G_0(r, r') \frac{\partial \psi_j^{(0)}(r')}{\partial n_1} \right]$$

$$+ \frac{1}{4\pi} \int_{c^2} ds' \left[ G_0(r, r') \psi_j^{(0)}(r') - G_0(r, r') \frac{\partial \psi_j^{(0)}(r')}{\partial n_2} \right],$$

(A8)

$$\psi_j^{(s)}(r) =$$

$$\frac{1}{4\pi} \int_{c^1} ds' \left[ G_1(r, r') \psi_j^{(s)}(r') - G_1(r, r') \frac{\partial \psi_j^{(s)}(r')}{\partial n_1} \right],$$

(A9)

$$\psi_j^{(p)}(r) =$$

$$\frac{1}{4\pi} \int_{c^2} ds' \left[ G_2(r, r') \psi_j^{(p)}(r') - G_2(r, r') \frac{\partial \psi_j^{(p)}(r')}{\partial n_2} \right],$$

(A10)

where $\psi_j^{(\alpha)}(r)$ represent the complex amplitudes in the host media $(j = 0)$, or in the scatterers’ volume, i.e. $j = 1, 2$, respectively. If the module of the electric incident field $|\psi_j^{inc}|$ is assumed to be known, for instance, then the scalar complex function $\psi_j^{inc}(r) = |\psi_j^{inc}| e^{-ik_0 r}$ represents the incident field under $s$-polarization. The incident electric field under $p$-polarization can be obtained by the plane-wave relationship of the fields to obtain $\psi_j^{inc}(r)$. The integral equations (A8)–(A10) are solutions of equation (A1). $ds$ denotes differential length element over $C_1$ or $C_2$. $G_j$ are the Green functions, which are solutions of the inhomogeneous Helmholtz equation

$$\nabla^2 G_j(r, r') + k_0^2 \varepsilon_j G_j(r, r') = -4\pi \delta(\mathbf{r} - \mathbf{r'}),$$

(A11)

They are evaluated as

$$G_j(r, r') = i\pi H_j^{(1)}(k_0 \sqrt{\varepsilon_j} |\mathbf{r} - \mathbf{r'}|),$$

(A12)

where $H_j^{(1)}(\cdot)$ denotes the Hankel function of the first class and order zero (one).

By means of the boundary conditions, equations (A2) and (A3), it is possible to decouple the integral equations (A8)–(A10), so they will depend only on the fields $\psi_j^{(\alpha)}(r')$ on each scatterer or contour. Solving numerically for $\psi_j^{(\alpha)}(r')$ and their normal derivatives over the boundaries $\frac{\partial \psi_j^{(\alpha)}(r')}{\partial n'}$, the fields can be calculated in any region of space.
A.2. Outputs of the method: near- and far-fields

A.2.1. Near-fields

After obtaining the source functions \( \psi_n^{(0)}(r') \) and \( \frac{\partial \psi_n^{(0)}(r')}{\partial n'} \), the near-fields can be calculated by using equations (A8)–(A10) together with the boundary conditions (A2) and (A3). Each pair of functions \( \psi_n^{(0)}(r') \) and \( \frac{\partial \psi_n^{(0)}(r')}{\partial n'} \) must be used for each respective contour.

A.2.2. Far-fields

The expression for the far scattered field can be approached from equation (A8) by making use of the asymptotic approximations of the Hankel functions when \( k_0 |r - r'| \gg 1 \).

\[
\psi_n^{\text{sc}}(r) \big|_{k_0 |r - r'| \rightarrow \infty} = \psi_n^{\text{sc}}(r) \big|_{k_0 |r - r'| \rightarrow \infty} = \frac{2}{\pi k_0 r} e^{-ik_0 r} \left[ T_{1,0}(\phi) + T_{2,0}(\phi) \right],
\]

(A14)

In this expression, the distance between cylinders has been supposed to be much smaller than the distance \( r, \) being \( r = |r| \) the first coordinate of the point \( r = (r, \phi) \) where the far-field is calculated. The functions \( T_{m,\alpha}(\phi) \) \((m = 1, 2)\) are the scattering amplitudes obtained by integral form, defined as

\[
T_{m,\alpha}(\phi) = \frac{i}{4} \int_{C_{\omega}} ds \left[ ik_0 (n' \cdot n_{\text{far}}(\phi)) \psi_n^{(0)}(r') + \frac{\partial \psi_n^{(0)}(r')}{\partial n'} \right],
\]

(A15)

where the limit \( n_{\text{far}}(\phi) = \frac{(r' - r)}{|r - r'|} \big|_{r \rightarrow \infty} \sim (\cos \phi, \sin \phi) \) has been defined.

With this formulation, the optical cross sections can be expressed as [70]:

\[
C_{\text{sc}a,\alpha} = \frac{2}{\pi k_0} \int_0^{2\pi} |F_n(\phi)|^2 d\phi,
\]

(A16)

\[
C_{\text{ext},\alpha} = \frac{4}{k_0} \text{Re} \left[ F_n(\theta = 0) \right],
\]

(A17)

\[
C_{\text{abs},\alpha} = C_{\text{ext},\alpha} - C_{\text{sc}a,\alpha},
\]

(A18)

where \( F_n(\phi) = \frac{\pi k_0}{\sqrt{1 - \frac{\sin^2 \phi}{\sin^2 \phi}}}. \) Note that the angle of forward scattering, \( \theta = \phi_0 + \pi - \phi, \) has been introduced in the argument of \( C_{\text{ext},\alpha}, \)—see figure 12. In the particular case of having a single wire, all the method can be reduced by setting only one scatterer as \( m = 1 \) above. In particular, \( m = 1 \) only in \( F_n \) and a radiation pressure’s cross section can also be defined through [70]

\[
C_{pr} = C_{\text{ext}} - (\cos \theta) C_{\text{sc}a},
\]

(A19)

where the following average must be taken

\[
(\cos \theta) C_{\text{sc}a} = \frac{1}{k_0} \int_0^{2\pi} |F_n(\phi)|^2 \cos \theta d\phi.
\]

(A20)

It is worth mentioning that the method has been implemented and tested to verify the convergence of the integrals. It was considered that the solutions had converged when the relative error was less than 0.05% between two consecutive discretizations. The method has been subjected to careful testing and extreme situations have been explored, such as \( r_1 \rightarrow 0, \) \( r_2 \rightarrow 0 \) or \( \epsilon_1 = \epsilon_0, \) \( \epsilon_2 = \epsilon_0 \) or \( \mu_1 = \mu_0, \) \( \mu_2 = \mu_0. \) In both sets of cases, the solution of the problem was naturally reduced to the one corresponding to a dielectric or magnetic solid wire, respectively.

A.3. 2D Mie calculations

In the case of a single wire, the results obtained by the integral method are easily comparable with the results given by the 2D Mie theory [3]. Furthermore, the Mie expansion allows identifying the resonant excitations [35]. The far-fields for each fundamental polarization can be characterized by

\[
C_{\text{ext},\alpha} = \frac{4}{k_0} \text{Re} \left\{ b_0 + 2 \sum_{l=1}^{\infty} b_l \right\},
\]

(A21)

\[
C_{\text{sc}a,\alpha} = \frac{4}{k_0} \left\{ |b_0|^2 + 2 \sum_{l=1}^{\infty} |b_l|^2 \right\},
\]

(A22)

\[
C_{\text{ext},p} = \frac{2}{x} \text{Re} \left\{ a_0 + 2 \sum_{l=1}^{\infty} a_l \right\},
\]

(A23)

\[
C_{\text{sc}a,p} = \frac{2}{x} \left\{ |a_0|^2 + 2 \sum_{l=1}^{\infty} |a_l|^2 \right\},
\]

(A24)

respectively, where \( x = k_0 R \) and the following coefficients are defined

\[
b_l = \frac{\eta_{l10} H_l^{(1)}(\eta_{l10} x) J_l(x) - J_l(\eta_{l10} x) H_l^{(1)}(x)}{\eta_{l10} J_l^{(1)}(\eta_{l10} x) H_l^{(1)}(x) - J_l(\eta_{l10} x) H_l^{(1)}(x)},
\]

(A25)

\[
a_l = \frac{J_l^{(1)}(\eta_{l10} x) J_l(\eta_{l10} x) - J_l(\eta_{l10} x) J_l^{(1)}(\eta_{l10} x)}{J_l^{(1)}(\eta_{l10} x) H_l^{(1)}(x) - J_l(\eta_{l10} x) H_l^{(1)}(x)},
\]

(A26)

where \( \eta_{l10} = \frac{\sqrt{\alpha} \eta_{l10}}{\sqrt{\alpha_{l10}}}. \) The electromagnetic resonances for \( s- \) and \( p- \)polarizations are related to the complex poles of the coefficients \( b_l \) and \( a_l \) respectively.

Then, in a way analogous to a quantum mechanical problem, a set of integral numbers identify the resonances. For three-dimensional (3D) spheres we deal with three quantum numbers: the radial number \( n, \) and the two angular momentum numbers \( l, m \) (do not confuse this \( m \) with the number of scatterers given above) [71]. For 2D spheres or circular wires, we deal only with two numbers: \( n, \) the radial number and \( l \) the azimuthal number. The (magnetic) angular momentum \( m \) is ignored since the problem has an ignorable coordinate, e.g. \( \varphi. \) Differently from the 3D problem of spheres, the angular mode \( l = 0 \) or monopole order can be excited in a dielectric 2D sphere. In spheres, the first allowed mode is \( l = 1.\)
A.4. Exact calculations of forces and torques

Consider the total time-averaged force \( \langle \mathbf{F}(t) \rangle \) exerted by an electromagnetic field to a closed surface \( S = S(V) \) that surrounds a regular volume \( V \) [1, 28]

\[
\langle \mathbf{F}(t) \rangle = \oint_{S(V)} \langle \mathbf{T}(\mathbf{r}, t) \rangle \cdot \hat{n} \, da
\]

where \( \hat{n} \) is the outward unit normal to \( S \) and \( \langle \mathbf{T}(\mathbf{r}, t) \rangle \cdot \hat{n} \) is the Maxwell stress tensor such that

\[
\langle \mathbf{T}(\mathbf{r}, t) \rangle \cdot \hat{n} = \pm \varepsilon_{\text{vac}} \varepsilon_{\text{vac}}(\mathbf{E}(\mathbf{r}) \cdot \hat{n}) \mathbf{E}^*(\mathbf{r}) + \mu_{\text{vac}} \mu_{\text{vac}}(\mathbf{H}(\mathbf{r}) \cdot \hat{n}) \mathbf{H}^*(\mathbf{r}) - \frac{1}{2} \varepsilon_{\text{vac}} \varepsilon_{\text{vac}} |\mathbf{E}(\mathbf{r})|^2 + \mu_{\text{vac}} \mu_{\text{vac}} |\mathbf{H}(\mathbf{r})|^2 \hat{n}
\]

and \( \hat{n} \) being the normal of \( S \) pointing to outward direction. \( S \) is considered as immersed in a medium of parameters \( \varepsilon_{\text{rb}}, \mu_{\text{rb}} \) that cannot support shear stresses [28, 72]. This relation for the optical forces is valid only for linear phenomena, and considering the scattering object as rigid [72].

In a similar way, an expression can be deduced for the net mechanical torque

\[
N(t) = \int_{S(V)} \langle \mathbf{T}(\mathbf{r}, t) \rangle \times \mathbf{r} \cdot \hat{n} \, da
\]

If a 2D problem is assumed with axial symmetry with respect to \( z \)-axis, the expression for the time-averaged force of equation (A27) can be reduced to (SI units)

\[
\langle d_{\text{ mech}} F_0 \rangle = \frac{1}{2} Re \left\{ \int_{C_l} \left[ \varepsilon_0 \varepsilon_{\text{vac}}(\mathbf{E}(\mathbf{r}) \cdot \hat{n}) \mathbf{E}^*(\mathbf{r}) + \mu_{\text{vac}} \mu_{\text{vac}}(\mathbf{H}(\mathbf{r}) \cdot \hat{n}) \mathbf{H}^*(\mathbf{r}) + \frac{1}{2} \varepsilon_0 \varepsilon_{\text{vac}} |\mathbf{E}(\mathbf{r})|^2 + \mu_{\text{vac}} \mu_{\text{vac}} |\mathbf{H}(\mathbf{r})|^2 \hat{n} \right] \, ds \right\}.
\]

In this case, the radius \( \mathbf{r} \) is always contained in the plane \( (x, y) \) and the surface integral is reduced to a curvilinear one through \( \int_{C_l} \int_{C_m} ds \int_{ds} dz \). The contour \( C_l \) must contain the scatterer \( l \) with its own normal \( \hat{n}_l \). In this work, \( l = 1, 2, 3 \) (see section 2); \( l = 1 \), 2 correspond to circles closing the wires 1 and 2, respectively, and \( l = 3 \) corresponds to a circle closing the entire dimer. As infinite cylinders are assumed, \( dz \to \infty \) and a net density of force \( d_{\text{ mech}} F_0 \) can be defined instead of the force \( F_0 \) itself. Similarly, a net density of torque \( d_{\text{ mech}} N_0 \) can be defined instead of torque, and the following equation is deduced from (A29)

\[
\langle d_{\text{ mech}} N_0 \rangle = \frac{1}{2} Re \left\{ \int_{C_l} \left[ \varepsilon_0 \varepsilon_{\text{vac}}(\mathbf{E}(\mathbf{r}) \cdot \hat{n}) \mathbf{r} \times \mathbf{E}^*(\mathbf{r}) + \mu_{\text{vac}} \mu_{\text{vac}}(\mathbf{H}(\mathbf{r}) \cdot \hat{n}) \mathbf{r} \times \mathbf{H}^*(\mathbf{r}) + \frac{1}{2} \varepsilon_0 \varepsilon_{\text{vac}} |\mathbf{E}(\mathbf{r})|^2 + \mu_{\text{vac}} \mu_{\text{vac}} |\mathbf{H}(\mathbf{r})|^2 \mathbf{r} \times \hat{n} \right] \, ds \right\},
\]

where \( d_{\text{ mech}} N_0 = d_{\text{ mech}} N_0 \hat{z} \) has dimensions of force. In the case of spin torques, the last term of equation (A31) can be eliminated if the contour \( C_l \) is simplified to a circle such that \( \mathbf{r} \times \hat{n}_l = 0 \).

Note that for plane waves, the condition (A28) is automatically satisfied. Note also that equations (A30) and (A31) are valid for both fundamental polarizations. In particular, the first (second) term of these equations always cancels out under polarization \( s (p) \) because of the orthogonality of the fields.

In the case of a single wire, the force density or radiation pressure density can also be calculated as [3]

\[
\langle d_{\text{ mech}} F \rangle = \frac{I_0}{c} C_{pr} \frac{k_0}{k_0}
\]

where \( C_{pr} \) is given by equation (A19) and \( I_0 \) is the intensity of the incident wave [70]. In the case of using the 2D Mie’s formulation, \( C_{pr} \) can be calculated by taking equation (A19) with the optical cross sections given by equations (A21) and (A22), and (A23) and (A24) for each polarization, respectively. To ensure the coherency of the methodology used here, all the spectra for single wires have been calculated using both integral and Mie formulations. Both methods have given the same results (not shown here).

An electric field amplitude \( |\mathbf{E}|^2 \) was assumed to calculate normalized mechanical densities. Then, the densities were scaled by the factor \( 4\pi \varepsilon_0 |\mathbf{E}|^2 \). In this way, the results are valid for use with arbitrary intensities of illumination. However, when using big incident powers or relatively long times in making measures, heating effects should be included in the problem [73, 74]. In practice, pulsed lasers can be used to limit heating in the particles. In this paper, neither the thermal fluctuations due to radiative heat transfer nor pulsed lasers are considered in the response.

In this work, the embedding medium is assumed to be air or vacuum, i.e. \( \varepsilon_{\text{rb}} = 1 \), \( \mu_{\text{rb}} = 1 \), and the systems are assumed to be made of silicon so that \( \varepsilon_{s1} = \varepsilon_{s2} = \varepsilon_{s1} = \mu_{s1} = 1 \) or \( \varepsilon_{s1} = \varepsilon_{s2} = \varepsilon_{s1} = \mu_{s2} = 1 \) for isolated wires or dimer systems, respectively.

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References

[1] Novotny L and Hecht B 2006 Principles of Nano-Optics (Cambridge: Cambridge University Press)
[2] Andrews D L 2007 Structured Light and Its Applications: An Introduction to Phase-Structured Beams and Nanoscale Optical Forces (New York: Elsevier)
[3] Bohren C F and Huffman D R 1998 Absorption and Scattering of Light by Small Particles (New York: Wiley)
[4] Dhokia K and Zemaněk P 2010 Rev. Mod. Phys. Opt. Lett. 82 1767–91
[5] Raziman T V, Wolke R J and Martin O J F 2015 Faraday Discuss. 178 421
[6] Nieto-Vesperinas M 2015 Opt. Lett. 40 3021–4
