Loss compensation symmetry in dimers made of gain and lossy nanoparticles

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Received 15 March 2017, revised 7 June 2017
Accepted for publication 13 September 2017
Published 5 February 2018

Abstract
The eigenmodes in a two-dimensional dimer made of gain and lossy nanoparticles have been investigated within an exact analytical approach. It has been shown that there are eigenmodes for which all Joule losses are exactly compensated by the gain. Among such solutions there are solutions with a new type of symmetry, which we refer to as loss compensation symmetry, as well as well-known parity–time (PT) symmetric solutions. Unlike PT symmetric ones, the modes with loss compensation symmetry allow one to achieve full loss compensation with significantly less gain that in the case of PT symmetry. This effect paves the way to new loss compensation methods in optics.

Keywords: PT symmetry, loss compensation, dimer, eigenmodes, plasmonics

1. Introduction

Often, for a deep understanding of physics as well as for many hi-tech applications, one needs to consider systems with small inner losses (high-Q systems). Eigenmodes in such systems are very pronounced, and one can think about possible new applications. Systems with small inner losses not only improve the performance of corresponding devices quantitatively but often show qualitatively new behavior. In particular, when the light is scattered by a single nanoparticle with small inner losses, an electric quadrupole mode can dominate the scattering spectrum over the dipole mode [1]. Moreover, unusual modes such as left-handed plasmonic [2] or chiral modes [3, 4] can be observed in systems with small losses. In dimers, i.e. systems consisting of two particles, an essentially new type of localized oscillation (‘plasmonic molecules’) can be seen for small losses and small distances between the particles [5, 6]. Low losses are very important for negative refractive index materials (NIM), magnetism at optical frequencies and transformational optics [7].

High-Q electromagnetic resonances can be easily discovered in the infrared (IR) frequency range, where almost transparent materials with high permittivity (silicon, germanium, etc) exist. In the mid-IR frequency range, a low-loss regime can be achieved with phonon–polariton resonances (SiC and others [8]) or with graphene [9, 10]. In the visible frequency band it is more difficult to find high-Q oscillations in nanoparticles, because typically in this range plasmon resonances have quite large optical losses. Hence, many interesting theoretical predictions are difficult to observe.

The idea of loss compensation using gain materials is now being widely discussed. Substantial progress has been achieved in loss compensation in metamaterials [11–13]. Of the various systems with loss compensation, parity–time (PT) symmetric systems exhibit very interesting effects, such as symmetry breaking and power oscillations [14–21]. Let us recall that,
in optics, PT symmetry means that permittivity of the system satisfies the following relation: $\varepsilon(x, y, z) = \varepsilon^*(−x, y, z)$ [14].

In this work we will present the results of an investigation of loss compensation in the general case of a dimer made of particles of the same shape but with arbitrary relation between gain and loss. For clarity we will consider two-dimensional (2D) oscillations in a dimer made of two 2D nanoparticles with permittivities $\varepsilon_G = \varepsilon' - i\varepsilon''_G (\varepsilon''_G > 0)$ and $\varepsilon_L = \varepsilon' + i\varepsilon''_L (\varepsilon''_L > 0)$ for gain and lossy nanoparticles, respectively. The geometry of the problem is shown in figure 1. This system can be considered as a generalization of the concept of a dipole nanolaser [22, 23].

Let us note that we are considering localized oscillation rather than propagating waves in waveguides. For this case one can find a general formulation of the eigenmode problem in [24–26]. Our approach can also be used to analyze eigenmodes in waveguides, but this is a topic for separate research. The question of stability of eigenmodes in plasmonic systems with loss compensation has been studied in [27, 28].

Let us also note that we consider general reasoning, and specific realization of the dimer is outside of scope of this work. However, several possible approaches to obtain gain nanoparticles are known [17, 29].

2. Material-independent eigenvalues and eigenmodes

By an exact analytical calculation of eigenmodes, we have shown that full loss compensation can be obtained not only for PT symmetric systems, i.e. when $\varepsilon''_G = \varepsilon''_L$, but also for the nonsymmetrical case $\varepsilon''_G \neq \varepsilon''_L$. We will refer to the eigenmodes in such asymmetrical systems as modes with loss compensation symmetry (LCS). Such modes allow one to achieve full compensation of optical losses even in the case $\varepsilon''_G \ll \varepsilon''_L$.

We define the eigenmodes of such a system as nontrivial solutions of Maxwell’s equations without any sources. As spectral parameters, we consider permittivity values of the system ($\varepsilon', \varepsilon''_G, \varepsilon''_L$). Such an approach is very powerful because eigenvalues and eigenmodes found within it do not depend on specific materials. The solution of a specific problem with specific materials can be easily discovered on the basis of known eigenmodes and eigenvalues. In this case, eigenfrequencies can be found from a specific dispersion relation between permittivity and frequency.

It is important to note that the use of classical Maxwell’s equations is only correct when the distance between the nanoparticles in the dimer is greater than a few nanometers, otherwise quantum effects need to be taken into consideration [30–32].

For particles that are small in comparison with the wavelength (nanoparticles), retardation effects are small and a quasistatic approach can be used. In this case, to find eigenmodes one should solve the Laplace equation for potential, satisfying the conditions of continuity for potential and a normal component of the electric displacement vector on all boundaries:

$$\mathbf{E} = -\nabla \varphi, \quad \Delta \varphi = 0,$$

where $\mathbf{E}$ is the electric field vector, $\varphi$ is the potential, $\nabla$ is the spatial gradient, $\Delta$ is the Laplacian and $S$ is the nanoparticle surfaces. Let us note that when considering a quasistatic problem radiation losses are not taken into account. It is very important that the real part of $\varepsilon$ as eigenvalues of (1) and (2) are negative numbers, which can be proved rigorously by potential theory [33, 34].

Knowing the eigenvalues of permittivity and eigenmodes of the problem (1) and (2), one can build a solution of any specific electrodynamics problem in the frequency domain [35].

In the case of 2D eigenmodes (which do not depend on the $z$ coordinate), to solve (1) and (2) it is convenient to introduce the bipolar coordinates $\theta$ and $\eta$, which are related to the Cartesian coordinates $x$ and $y$ by the following relations [36]:

$$\eta = \text{atanh} \left( \frac{2\eta}{\eta^2 + 1} \right),$$

$$\theta = \text{atan} \left( \frac{2\eta}{\eta^2 + 1} \right).$$

In (3), $2f$ is the distance between foci of the bipolar coordinate system. Hence, an arbitrary solution of the Laplace equation (1) can be expressed as a sum of the functions $e^{(2n+1)i\theta} x^n, n = 1, 2, \ldots$ [36]. The boundaries of particles of equal size are defined by the equations $\eta = \pm \eta_0 (\eta_0 > 0)$, which correspond to the radius $f/\sinh \eta_0$ and the distance between the particle centers, $2f/\coth \eta_0$. The particle permittivities are $\varepsilon_G$ and $\varepsilon_L$, respectively, while the permittivity of the surrounding medium is taken to be $\varepsilon_m = 1$ (vacuum).

The potential distribution outside and inside the particles can be written in the form

$$\varphi_G = a e^{in}, \quad \varphi_L = d e^{-in}, \quad \varphi_{out} = be^{in} + ce^{-in},$$

where $\varphi_G, \varphi_L$ and $\varphi_{out}$ are the potentials inside gain and lossy particles and outside them, respectively. The choice of this form of solution is associated with the requirement to limit the potential in space. The unknown coefficients $a, b, c, d$ and $n$ can be found by applying the boundary conditions (2). In (4), and below for brevity, we omit the factors $\cos (n\theta)$ or $\sin (n\theta)$ in the potentials. Substituting (4) into (2), the following exact dispersion relation can be obtained:
\((\varepsilon_L - 1)(\varepsilon_G - 1) = (\varepsilon_L + 1)(\varepsilon_G + 1)e^{4\eta n p},\) \hspace{1cm} (5)

which is valid for each azimuthal number \(n\). If (5) is valid, the following important relations between coefficients in (4) can be easily obtained:

\[
\begin{align*}
\frac{a}{d} &= (1 - \varepsilon_L)(1 + \varepsilon_G)^{-1}e^{-2\eta n p}, \\
\frac{b}{d} &= 0.5(1 - \varepsilon_L)e^{-2\eta n p}, \\
\frac{c}{a} &= 0.5(1 - \varepsilon_G)e^{-2\eta n p}.
\end{align*}
\hspace{1cm} (6)

It is also very important that one can strictly prove that any eigensolution of (1) satisfies the condition of full loss compensation, that is:

\[
\int_{V_G} \varepsilon''_G|\mathbf{E}(r)|^2 \, dr = \int_{V_L} \varepsilon''_L|\mathbf{E}(r)|^2 \, dr,
\hspace{1cm} (7)
\]

where \(V_G\) and \(V_L\) are the volumes of gain and lossy nanoparticles. Thereby if one attributes effective permittivity [37] to the whole system, its imaginary part will be equal to zero, so our system is similar to pseudo-Hermitian systems [38].

Let us note that in a case with retardation, an additional term appears in the right-hand side of (7), which corresponds to radiative losses in the system. To satisfy (7), the value of \(\varepsilon''_G\) can become bigger with increasing radiative losses. In this work we make use of the quasistatic approximation in which radiative losses are neglected.

First of all, let us consider the PT symmetric system with

\[
\varepsilon_G = \varepsilon' - i\varepsilon'', \quad \varepsilon_L = \varepsilon'_L,
\hspace{1cm} (8)
\]

where \(\varepsilon'\) and \(\varepsilon''\) are real numbers. Substituting (8) into (5), one can obtain the following relation between the real and imaginary parts of permittivity:

\[
[\varepsilon' + \coth(2\eta n p)]^2 + \varepsilon''^2 = \frac{1}{\sinh^2(2\eta n p)}.
\hspace{1cm} (9)
\]

Following from equation (9), the dispersion curve for a PT symmetric system in coordinate space \(\varepsilon'\), \(\varepsilon''\) is a circle with radius \(1/\sinh(2\eta n p)\) with its center at \(\varepsilon' = -\coth(2\eta n p), \quad \varepsilon'' = 0\).

If \(\varepsilon'' < 1/\sinh(2\eta n p)\), the PT symmetric system has PT symmetric eigenmodes:

\[
\varphi(x) = \varphi^*( -x).
\hspace{1cm} (10)
\]

The specific form of (10) is given below (see the structure of potential given by (18)). However, if \(\varepsilon'' > 1/\sinh(2\eta n p)\), the PT symmetric system (8) has no eigenmodes that are finite in space. It is important to note that the absence of eigenmodes after PT symmetry breaking in our geometry does not contradict [14] or other works on PT symmetry in coupled waveguides. This is because we consider localized eigenmodes with finite fields while modes in the PT broken phase (see [14] for example) are propagating and divergent. More importantly, in our case we have finite solutions with new symmetry in the region where PT symmetric solutions are absent.

For an asymmetric system \((\varepsilon_L \neq \varepsilon'_L)\), eigenmodes only exist for one specific value of the real part of permittivity (for each \(n\)), which is defined by geometrical parameters only:

\[
\varepsilon_{\text{LCS}} = -(\varepsilon'' + 1)/(\varepsilon'' - 1),
\hspace{1cm} (11)
\]

while the imaginary parts of the permittivity for gain and lossy nanoparticles can vary relative to each other, but their product is fixed:

\[
\varepsilon_{\text{G,LCS}}'' = 4\varepsilon''/(\varepsilon'' - 1)^2.
\hspace{1cm} (12)
\]

It follows from (12) that in our dimer full loss compensation is possible for an arbitrary value of the imaginary part of permittivity in a lossy particle. Moreover, the greater \(\varepsilon_{\text{LCS}}''\), the smaller the \(\varepsilon_{G,LCS}''\) required for full loss compensation, because they depend on each other inversely. This effect results from asymmetry of the field distribution between gain and lossy particles, so when \(\varepsilon_{G,LCS}''\) gets bigger, the amplitude of the field in the lossy particle decreases relative to the active particle (see figure 4).

One can show that the eigenmodes of an asymmetrical system with permittivities given by (11) and (12) have a non-trivial symmetry:

\[
\varphi(x) = \varphi^*( -x) \begin{bmatrix} \theta(-x) \sqrt{\varepsilon''_G/\varepsilon''_L} \\ +\theta(x) \sqrt{\varepsilon''_L/\varepsilon''_G} \end{bmatrix}, \quad |\eta| > \eta_0,
\hspace{1cm} (13)
\]

where \(\theta(x)\) is the Heaviside step function. We will refer to this symmetry as LCS. For the PT symmetric case \(\varepsilon''_L = \varepsilon''_G\), this symmetry is reduced to PT symmetry.

The full spectrum of eigenmodes of the system under consideration is shown in figure 2 for particles with a radius of 10nm and a distance between their centers of 28nm.

As can be seen in figure 2, the spectrum of PT symmetric modes indeed lies in the plane \(\varepsilon''_G = \varepsilon''_L\), while the spectrum of LCS modes lies in the perpendicular plane \(\varepsilon'' = \text{const}\). It is worth mentioning that the branches of the dispersion curve touch each other at one point (marked as the critical point in figure 2), allowing one to speculate about spontaneous breaking
of PT symmetry at this point and transition to solutions with LCS. The values of permittivity \( \varepsilon_L \), \( \varepsilon_G \) of particles for this critical point are defined only by geometrical parameters of the system and can be easily deduced from (11) and (12):

\[
\begin{align*}
\varepsilon_L &= (2i^{e^{2\eta_p}} - (e^{4\eta_p} + 1)) / (e^{4\eta_p} - 1), \\
\varepsilon_G &= (\varepsilon_L^*).
\end{align*}
\]  

(14)

In figure 2, the eigenmodes are shown for \( n = 1 \) only. Eigenmodes with higher azimuthal number \( n \) will have a similar shape, and the real part of the permittivity of particles \( \varepsilon' \) will tend to minus unity in accordance with (11).

Now let us consider the spatial distribution of potentials for PT symmetric eigenmodes. PT symmetry of potential means that

\[
\varphi(x) = \varphi^*(−x).
\]  

(15)

From (15), it follows immediately that the real part of the potential should be symmetric while the imaginary part should be antisymmetric. From (15), it also follows that in (4) one should put

\[
a = a^*.
\]  

(16)

It can be demonstrated that (16) is true only when (8) is satisfied, i.e. the potential can have PT symmetry only if the system permittivity has such symmetry itself. Extracting the real and imaginary parts of \( a \), \( a = a' + ia'' \) (where \( a' \) and \( a'' \) are real numbers), from (6) and (16), one can obtain

\[
a'' = -i(F - 1)/(F + 1) a', \quad F = 1 - \varepsilon_L e^{-2\eta_p}.
\]  

(17)

It is interesting to note that the imaginary unit in (17) is cancelled by the factor \( (F - 1)/(F + 1) \), and \( a'' \) remains real for all PT eigenmodes except \( \varepsilon_L^G = \varepsilon''_L = 0 \). The potential at any point on a PT symmetric branch can be written in the form

\[
\varphi = a' \varphi^s + ia'' \varphi^a,
\]  

(18)

where the symmetric \( \varphi^s \) and antisymmetric \( \varphi^a \) parts of the potential are real and universal and can be found from (4) by the substitution

\[
a = 1, \quad b = 0.5(1 - \varepsilon_L) e^{-2\eta_p}, \\
c = 0.5(1 - \varepsilon_G) e^{-2\eta_p}, \quad d = 1,
\]  

(19)

and

\[
a = 1, \quad b = -0.5(1 - \varepsilon_L) e^{-2\eta_p}, \\
c = 0.5(1 - \varepsilon_G) e^{-2\eta_p}, \quad d = -1,
\]  

(20)

respectively. For pure real permittivities (marked as a cross and a star in figure 2) either \( a'' \) or \( a' \) is equal to zero, and eigenmodes becomes symmetric or antisymmetric relative to the parity transformation \( x \to -x \). The spatial distribution of \( \varphi^s \) and \( \varphi^a \) is shown in figure 3.

Now let us consider asymmetrical systems with \( \varepsilon_L \neq \varepsilon_G \) and related LCS modes. Since full loss compensation exists for any solution of (1), one can find an additional relation between \( a \) and \( d \) in (4):

\[
\varepsilon_G^a |d|^2 - \varepsilon_L^s |d|^2 = 0.
\]  

(21)

By choosing an appropriate arbitrary phase, the solution of (21) and (6) can be written as

\[
a = a' + ia'', \quad d^* = a'/\kappa,
\]  

(22)

where

\[
a'' = -i(F/\kappa - 1)/(F/\kappa + 1) a', \quad \kappa = \sqrt{\varepsilon''_L/\varepsilon''_G}.
\]  

(23)

Here again, despite there being an imaginary unit in (23), \( a'' \) remains real for all LCS eigenmodes. Other coefficients in (4) are defined by (6). For the general case (22), the potential inside the particles satisfies the condition of LCS symmetry:

\[
\varphi(x) = \varphi^*(−x) [\varepsilon_0 (−x + \theta(x))/\kappa], \quad |\eta| > \eta_0.
\]  

(24)

The potential outside the particles \( |\eta| < \eta_0 \) does not satisfy (24). Let us stress that equations (22)–(24) transform to (16), (17) and (15) for a PT symmetric system because for that case \( \kappa = \sqrt{\varepsilon''_L/\varepsilon''_G} = 1 \).

The spatial distribution of the potential for the LCS mode is shown in figure 4 for the case of a substantial difference between \( \varepsilon''_L \) and \( \varepsilon''_G \) in nanoparticles: \( \varepsilon_G = -1.06 - 0.156i \) and \( \varepsilon_L = -1.06 + 0.85i. \)

It can be seen from figure 4 that the amplitude of the potential (and therefore the field) in the left (gain) particle is much higher than in the right (lossy) one. Meanwhile, the modulus of the imaginary part of the permittivity in the right particle is much higher than in the left one \( \varepsilon''_L = 0.85 \gg \varepsilon''_G = 0.156 \). In figure 4, it is difficult to trace LCS (19). However, if one plots the distribution of Joule losses \( \sim \varepsilon''(\mathbf{r}) |\mathbf{E}(\mathbf{r})|^2 \) in space (see figure 5), the LCS and full loss compensation becomes evident.
Let us note that we consider only the case with equal real parts of the particle permittivities. If one were to consider a more general case with $\varepsilon_G = \varepsilon'G - i\varepsilon''G$ ($\varepsilon''G > 0$), $\varepsilon_L = \varepsilon'_L + i\varepsilon''_L$ ($\varepsilon''_L > 0$) then a 2D surface in a 4D space with coordinates $\varepsilon'_G, \varepsilon''_G, \varepsilon'_L, \varepsilon''_L$ would be a solution.

3. Possibility of application to real systems

From figure 2 one can see that for an ‘interesting’ regime of LCS modes ($\varepsilon''_L \gg \varepsilon''_G$), a specific relation between the imaginary and real parts of the permittivity of a lossy particle is needed. For this regime in particular, the imaginary part of the permittivity should be of the same order of magnitude as the real one, with the absolute value of the real part close to 1. This condition can be satisfied, for example, for gold. However, a promising plasmonic material, TiN (see e.g. [8, 39–41]), would do better because of a bigger imaginary part of the permittivity in the visible part of the spectrum. In figure 6, one can see both material-independent PT and LCS modes for different radii and permittivities of TiN (wavelengths 470–600 nm) and Au (wavelengths 470–540 nm). The distance between the particles is 140 nm.

From the wave equation for the vector potential:

$$\Delta A + k_0^2 \varepsilon A = -ik_0\varepsilon \nabla \varphi,$$  \hspace{1cm} (27)

one can see that $A = O(k_0)$. Therefore, (26) can be simplified to:

$$\Delta \varphi = 0, \hspace{1cm} [\varepsilon \partial \varphi/\partial n]_S = O(k_0^2).$$  \hspace{1cm} (28)

From (28), it follows that retardation effects for nanoparticles only result in small changes in the eigenvalue problem (1) and (2), and therefore the solutions we have found for PT and LCS modes are also valid for the case with retardation. Numerical simulations of the full 3D system of Maxwell equations confirm this fact. Therefore, new LCS modes can be observed at telecoms and visible wavelengths.

4. Conclusion

In conclusion, the problem of 2D localized eigenmodes in a dimer made of gain and lossy nanoparticles has been solved analytically. The located eigenmodes appear when all optical
losses in the first particle are compensated by amplification of the optical fields in the second particle. It has been demonstrated that together with PT symmetric modes in a PT symmetric system ($\varepsilon'_G \neq \varepsilon'_L$), there are new types of modes for an asymmetric system with $\varepsilon''_G \neq \varepsilon''_L$. We refer to these as modes with LCS. These modes require a small absolute value of the imaginary part of the permittivity. This feature of LCS modes paves the way to new methods of loss compensation.

In addition, all modes are characterized by the mixing of symmetric and antisymmetric modes which exist in nanoparticles without losses.

Acknowledgments

The research has been supported by the Advanced Research Foundation (contract no. 7/004/2013-2018). Authors acknowledge financial support from the Russian Foundation for Basic Research (grant no. 14-02-00290 and no. 15-52-52006). VVK acknowledges support from the MEPhi Academic Excellence Project (Contract No. 02.a03.21.0005).

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