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**PAPER**

Disorder effects on the coupling strength of coupled photonic crystal slab cavities

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¹ Author to whom any correspondence should be addressed.**E-mail:** juan.vasco@epfl.ch and vincenzo.savona@epfl.ch**Keywords:** photonic crystals, coupled cavities, disorder**Abstract**

We study the effects of disorder on the coupling strength of coupled photonic crystal slab cavities by considering fully-3D electromagnetic calculations. Specifically, we investigate two coupled $L3$ cavities at 30° and 60° configurations, where the coupling strength J (or photon hopping) is extracted from the simulations in the presence of disorder. We found that the relative fluctuations of the photon hopping are more sensitive to disorder effects than the corresponding fluctuations in the eigenfrequencies of the coupled cavities. Furthermore, for the typical range of disorder in state-of-the-art devices, the J fluctuations are found to increase linearly as a function of the disorder amplitude. This allows one to set upper bounds to the amplitude of fabrication imperfections, for which the coupling predicted by design can still be expected, on average, in a fabricated device.

1. Introduction

Photonic crystals (PhCs) have been the focus of intense investigations over the last three decades, thanks to the unique possibility they offer to engineer the density of states of the electromagnetic field and, consequently, the flow of light [1, 2]. The maturity subsequently achieved in semiconductor nano-fabrication technology has led to a plethora of PhC-based device concepts that may have large impact in future integrated photonic platforms [3–7]. In analogy with electron states in crystals, the electromagnetic modes in a PhC form bands. When in presence of a forbidden bandgap, defects in PhCs can be engineered to give rise to confined light modes, typically in 0D (cavities) or 1D (waveguides) [8]. In particular, two-dimensional PhCs made of a triangular lattice of holes on a dielectric slab, have emerged as a paradigm for various functionalities, as they enable the realization of cavities and waveguides with various geometries and figures of merit, to be used as building blocks of more complex photonic devices. Important recent examples are large-scale integration of all-optical memories [9], all-optical PhC logic gates and switching [10–12], strong coupling between distant PhC nanocavities [13], optical sensing [14, 15] and wide-band slow light coupled cavity waveguides [16, 17]. Moreover, recent advances in PhC optimization have shown that figures of merit—such as Q -factors or broadband slow light—can be dramatically improved with simple local changes to the nominal PhC structure [17–24].

Even with the most advanced nano-fabrication resources, disorder in the form of small deviations from the nominal geometry is always present, to some extent, in fabricated PhC structures. The effects of structural disorder on the properties of PhC structures have been extensively studied in the case of cavities [25–27] and waveguides [28–31], as well as in coupled cavity systems [32–34]. Most of these studies have been focusing on the effect of disorder on the resonant frequencies of the electromagnetic modes and on their quality factors. The question of how disorder affects the coupling induced by spatial proximity in the case of two resonant PhC structures, remains yet to be addressed. More specifically, if the coupled cavity system is described by the simplest coupled-mode model—with resonant frequencies $\omega_{1,2}$, respectively, for the two cavities, and a photon hopping rate J —we are interested in the fluctuations of J for a given statistical ensemble of disorder realizations.

In this work we investigate the disorder effects on the coupling strength of coupled PhC cavities. By means of the guided mode expansion method (GME) and a two coupled-mode model, we compute the coupling strength

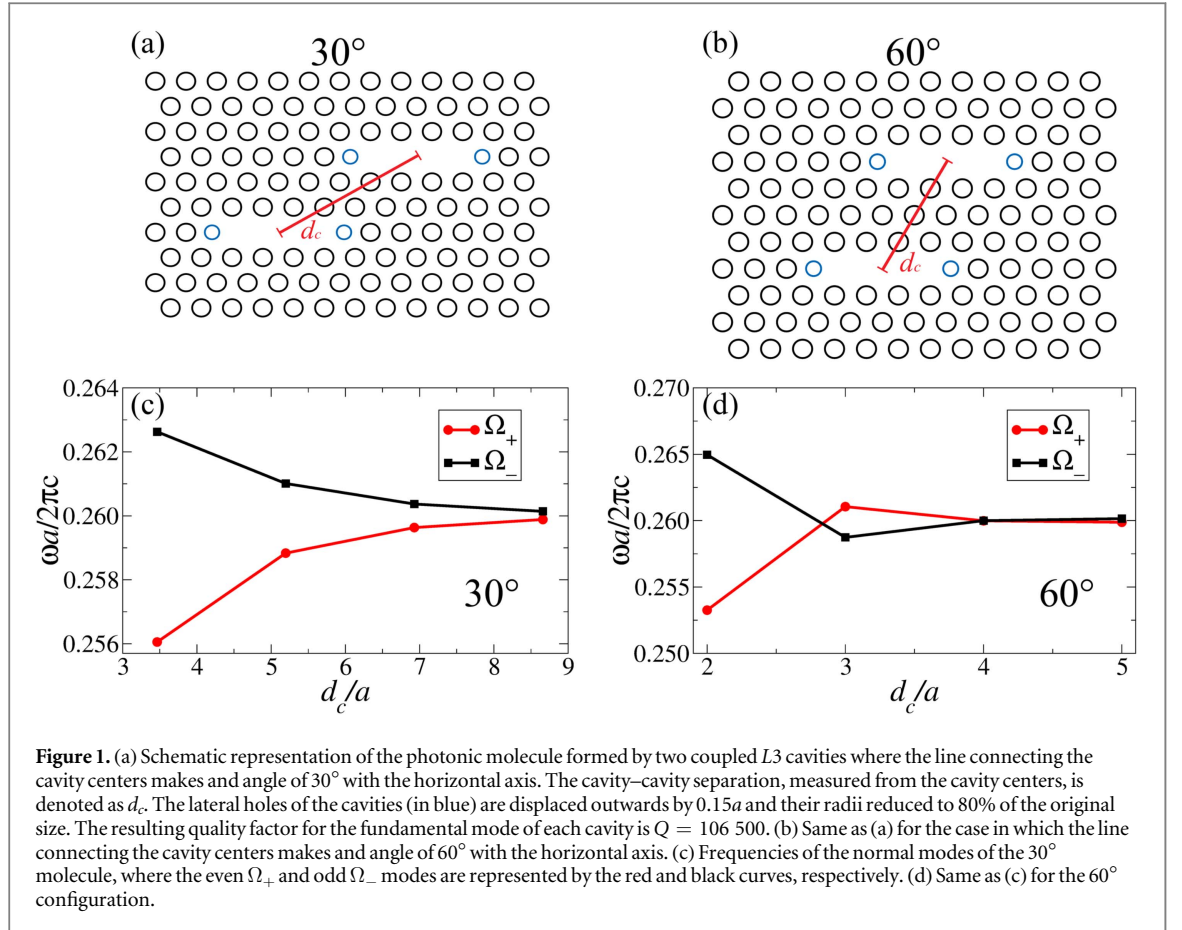


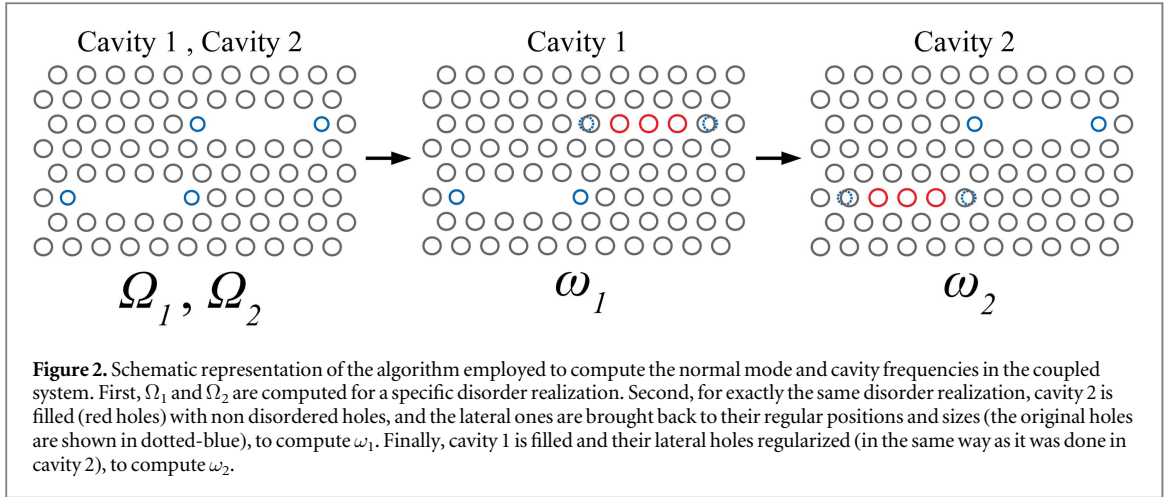
Figure 1. (a) Schematic representation of the photonic molecule formed by two coupled L3 cavities where the line connecting the cavity centers makes an angle of 30° with the horizontal axis. The cavity–cavity separation, measured from the cavity centers, is denoted as d_c . The lateral holes of the cavities (in blue) are displaced outwards by $0.15a$ and their radii reduced to 80% of the original size. The resulting quality factor for the fundamental mode of each cavity is $Q = 106\,500$. (b) Same as (a) for the case in which the line connecting the cavity centers makes an angle of 60° with the horizontal axis. (c) Frequencies of the normal modes of the 30° molecule, where the even Ω_+ and odd Ω_- modes are represented by the red and black curves, respectively. (d) Same as (c) for the 60° configuration.

J of two coupled L3 PhC cavities in the presence of disorder, i.e., in the regime where the two cavities have different resonant frequencies. We find that the relative fluctuations of J with respect to their mean values, $\delta J / \langle J \rangle$, are more sensitive to disorder than the relative fluctuations of the normal mode frequencies, $\delta \Omega / \langle \Omega \rangle$, of the coupled cavity system. We finally establish the scaling law of $\delta J / \langle J \rangle$ as a function of the disorder parameter and set an upper bound to the amplitude of random imperfections in the system, in order for the nominal coupling to be realized on average, i.e. $\delta J / \langle J \rangle \ll 1$. The present results are of particular relevance for the design of state-of-the-art integrated PhC devices and for the rapidly growing research on quantum many-body phenomena in photonic arrays [35–40].

The paper is organized as follows. In section 2 we discuss the resonant modes of the ideal (i.e. non disordered) system of two coupled PhC cavities, and explain the procedure to compute the coupling strength J , by combining GME with a two coupled-mode model in the presence of disorder. In section 3, we present results for the coupled cavity system in presence of disorder and discuss the scaling law for the relative fluctuations $\delta J / \langle J \rangle$ and $\delta \Omega / \langle \Omega \rangle$. Finally, we draw conclusions in section 4.

2. System and methods

We consider the system of two coupled L3 PhC cavities, as schematically shown in figure 1, which we will refer to as a photonic molecule. Two specific configurations are investigated: the one in which the line connecting the centers of the cavities makes an angle of 30° with respect to the horizontal axis, figure 1(a), and the one in which this angle is 60° , figure 1(b). The 30° configuration is the most commonly adopted, as it results in sizable coupling strength over a wide range values of the inter-cavity distance. On the other hand, as we will show, the 60° configuration presents with an oscillatory behavior of the coupling as a function of distance, resulting in a ‘soft spot’ at a distance of around four times the lattice parameter, where the coupling is almost vanishing. This particular configuration makes it possible to extend the present study to the case where the weak disorder limit breaks down and the fluctuations in the coupling strength become as large as its average value. The cavity–cavity distance, measured from the cavity centers, is denoted by d_c . We consider parameters that are typical for silicon PhCs, i.e., refractive index $n = 3.46$, hole radii $r = 0.25a$ and slab thickness $d = 0.55a$ where a is the lattice parameter of the underlying hexagonal PhC lattice. With this choice, if the lattice parameter is set to $a = 400$ nm, the resonant wavelength of the L3 cavity lies around $\lambda = 1.55$ μm . We employ a partially



optimized design of the $L3$ cavities where the lateral holes (blue holes in figures 1(a) and (b)) are displaced outwards along the horizontal direction by $s = 0.15a$ and their radii decreased to $r' = 0.8r$. In this way, the nominal (unloaded) quality factor of a single $L3$ mode is $Q = 106\,500$. The normal modes of the PhC molecule are computed using the GME approach, in which the Bloch modes of the PhC are expanded on the basis of guided modes of the effective homogeneous semiconductor slab [41]. For the simulations, periodic boundary conditions are assumed, with a rectangular supercell of lateral dimensions $20a \times 7\sqrt{3}a$ and $17a \times 8\sqrt{3}a$ for the 30° and 60° cases, respectively. For the expansion onto guided modes, a momentum cutoff $a|\mathbf{G}|_{\max} = 20$ is used, and only the first TE guided mode of the slab was included in the GME expansion. We have carefully verified the convergence of the results with respect to these simulation parameters. The frequencies of the two normal modes originating from the coupling between the two fundamental $L3$ cavity modes are shown for the ideal 30° configuration in figure 1(c), and for the 60° one in figure 1(d). In the absence of disorder, these modes are, respectively, even and odd with respect to the inversion symmetry around the middle point of the structure. A coupling arises from the overlap between cavity modes, giving rise to a normal mode splitting Δ which depends on the cavity–cavity separation d_c . Interestingly, spatial oscillations in the tails of the overlapping cavity modes can give rise to a non-monotonic dependence of Δ as a function of d_c . This phenomenon is evidenced in figure 1(d) for the 60° case, where the Δ clearly becomes very small at $d_c = 4a$ and increases from $d_c = 4a$ to $d_c = 5a$. Eventually, for large cavity–cavity separation, both normal modes tend to the single frequency value of the fundamental $L3$ cavity mode [42, 43].

Fabrication disorder in the PhC structure is modeled in terms of independent and non-correlated random fluctuations of all hole positions and radii within the supercell [26, 44]. The probability distribution of the random fluctuations is chosen to be Gaussian with the corresponding standard deviation σ taken as our disorder parameter, in line with previous experimental and theoretical characterizations of intrinsically disordered PhCs [19, 28, 31, 45, 46]. When disorder is present, extrapolating the value of the coupling strength J from the GME simulation is not straightforward. Indeed, disorder produces both a fluctuation in the resonant frequencies of the two uncoupled cavities and a fluctuation in the coupling strength J . In order to extract the value of J from the simulation we adopt the following procedure based on a coupled-mode theory. The two normal modes of the molecule are modeled as the eigenmodes of the 2×2 matrix

$$M = \begin{pmatrix} \omega_1 & J \\ J & \omega_2 \end{pmatrix}, \quad (1)$$

where ω_1 and ω_2 are the (yet unknown) resonant frequencies of the two uncoupled cavities. The idea consists in determining—for each given realization of disorder—the value of J for which the eigenvalues of the matrix M are closest to the GME-computed normal mode frequencies, which we denote by Ω_1 and Ω_2 (assuming $\Omega_1 < \Omega_2$). To this purpose, we need to compute the values of the uncoupled resonant frequencies ω_1 and ω_2 , for the very same disorder realization. The values Ω_1 , Ω_2 , ω_1 , and ω_2 are all obtained from GME calculations, following the steps sketched in figure 2. For a given disorder realization, we first use GME to simulate the two coupled cavities, thus obtaining the eigenfrequencies Ω_1 and Ω_2 . Then, for the same disorder realization, we restore the missing holes of cavity 2 (red circles) and bring back the nearest side holes to their regular positions and sizes. This corresponds to effectively removing cavity 2 from the given disordered realization. Simulating this new configuration with GME provides the uncoupled frequency ω_1 of cavity 1. Finally, by following the same steps as for cavity 1, we compute the frequency ω_2 . One important question concerns the sensitivity of ω_1 and ω_2 to disorder in the added holes. We would expect that disorder on the three restored holes of cavity 1 (2) should have minor influence on the GME-computed frequency of cavity 2 (1), as the restored holes reside far

from the position where the resonant cavity mode is confined. We have checked this assumption by actually considering several disorder realizations for the restored holes. It turns out that disorder on the three restored holes produces fluctuations in the computed resonant frequencies which are always negligible with respect to the main fluctuations induced by disorder on the whole supercell. We can therefore safely avoid to average over several realizations of disorder on the restored holes and simply introduce them in their nominal positions and radii. In all results shown below, we have considered 500 independent disorder realizations and we have checked that the first and second moments of the computed statistical distributions are well converged for this number of realizations. Once the frequencies $\Omega_1, \Omega_2, \omega_1$, and ω_2 are known for a given disorder realization, the coupling strength J is determined by fitting the eigenfrequencies of the coupled-mode model (1) to these values. This is achieved by minimizing the function

$$F(J) = \sqrt{[\lambda_1(J) - \Omega_1]^2 + [\lambda_2(J) - \Omega_2]^2}, \quad (2)$$

where $\{\lambda_1(J), \lambda_2(J)\}$ are the eigenvalues of the matrix M . It may be argued that the coupling in the photonic molecule under consideration is not adequately modeled by a coupled-mode theory with only one mode per cavity, and that the effect of the presence of other resonant modes plays a role. We ruled out this possibility by generalizing the procedure described above, to include higher cavity modes in a coupled-mode theory with a larger number of modes. The generalized approach produced values of J that are essentially unchanged with respect to the simple two-mode approach, thus confirming the validity of this latter.

3. Results

We show in figures 3(a)–(d) the probability density function (PDF) of the normal mode frequencies in the 30° and 60° configurations, as computed with GME for a disorder amplitude $\sigma = 0.005a$ and two different values of d_c ; the red lines are fits to the Gaussian distribution, with average $\langle\Omega\rangle$ and standard deviations $\delta\Omega$. The corresponding PDFs of the coupling strength J , and the associated Gaussian fits, are displayed in figures 3(e)–(h) for the 30° and 60° molecules.

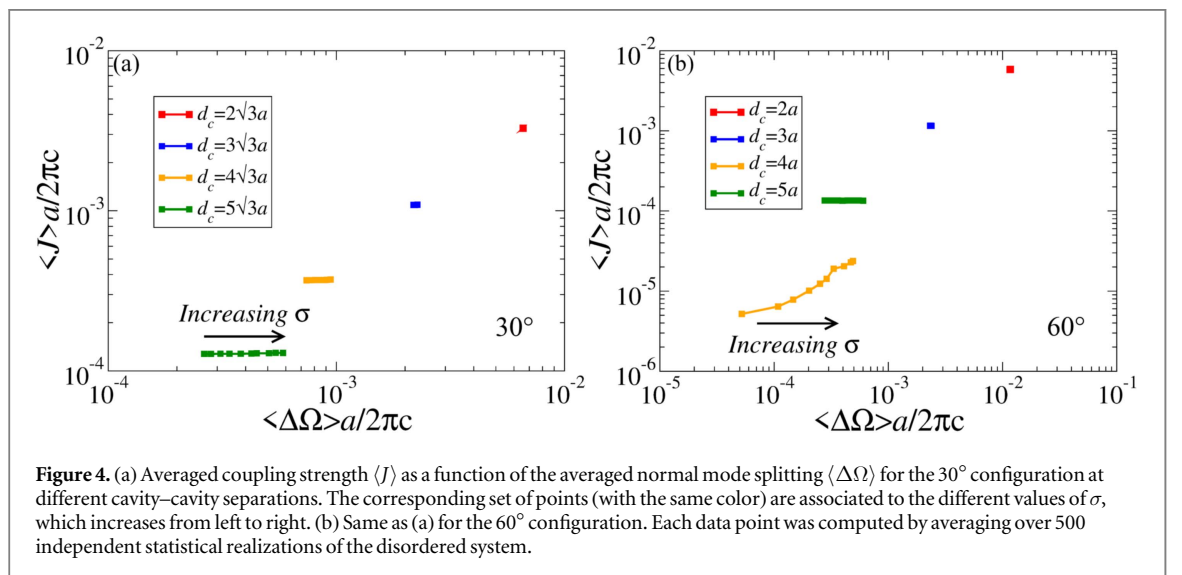
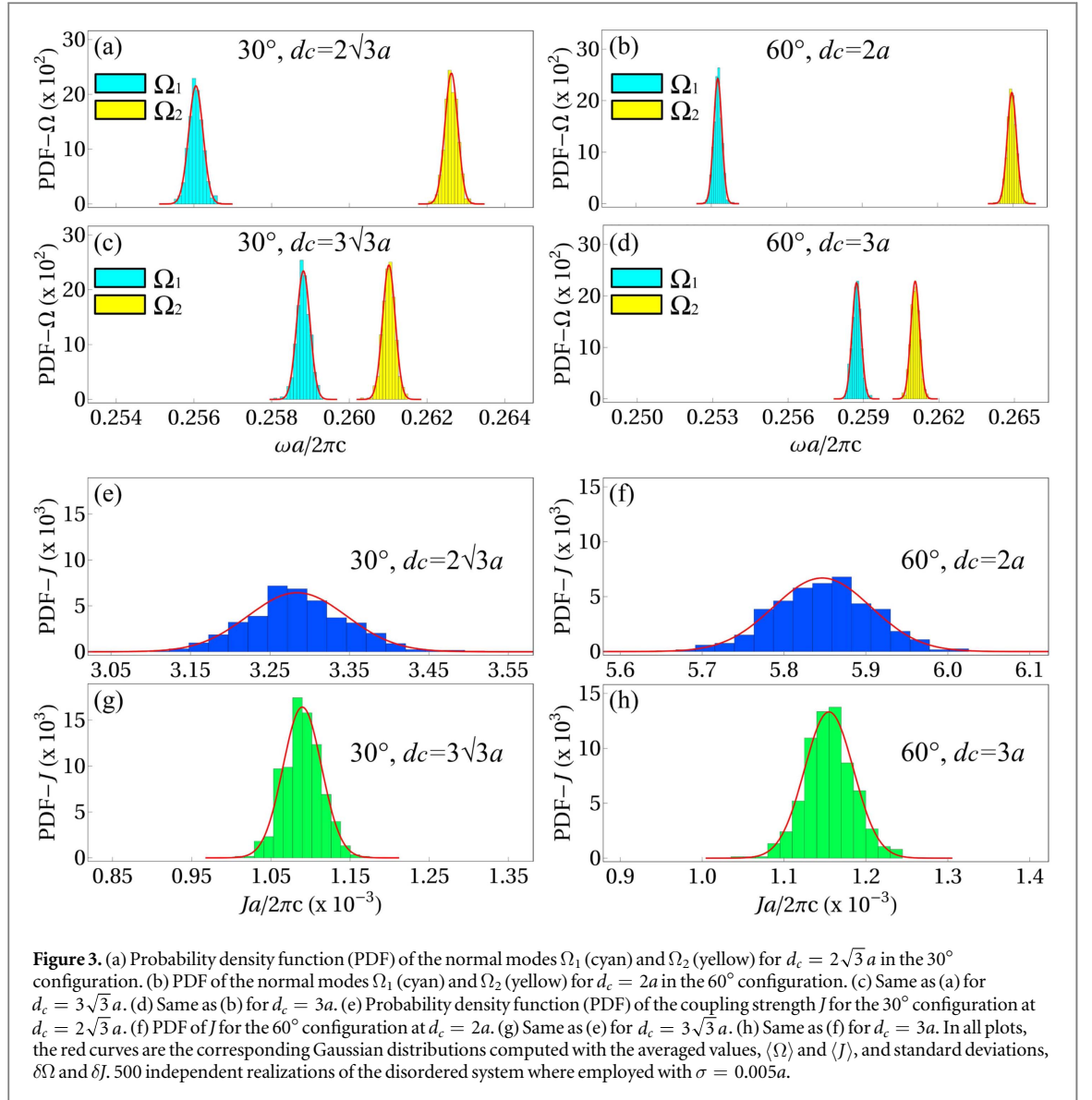
The link between the averaged coupling strength $\langle J \rangle$ and averaged normal mode splitting $\langle \Delta\Omega \rangle$ is shown in figures 4(a) and (b), for the 30° and 60° molecules, respectively, in log–log scale. We have considered values of the disorder amplitude ranging between $\sigma = 0.001$ and $\sigma = 0.01$, consistent with the typical accuracy achieved in state-of-the-art semiconductor fabrication [19, 46]. The coupling strength $\langle J \rangle$ increases with increasing $\langle \Delta\Omega \rangle$, as expected. For a given value of $\langle J \rangle$, disorder induces an overall increase in $\langle \Delta\Omega \rangle$, which is more pronounced for small values of $\langle J \rangle$. This increase is known to occur in a coupled-mode model when Gaussian distribution of the uncoupled frequencies is assumed, with a width much smaller than the normal mode splitting (i.e. in the weak disorder regime) [47]. From the plot it can be inferred that, in the limit $\sigma \rightarrow 0$ the relation between $\langle J \rangle$ and $\langle \Delta\Omega \rangle$ becomes linear, as expected from coupled-mode theory.

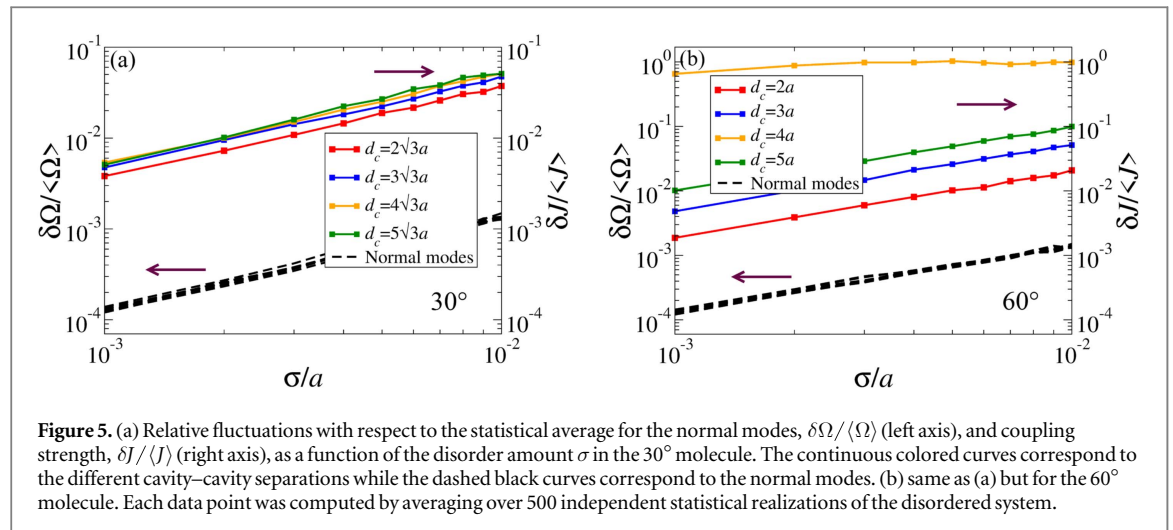
The relative fluctuations $\delta\Omega/\langle\Omega\rangle$ and $\delta J/\langle J \rangle$, are shown in figures 5(a) and (b) for the 30° and 60° cases, respectively, as a function of the disorder amplitude. On a double logarithmic scale, we clearly identify a linear dependence of $\delta J/\langle J \rangle$ and $\delta\Omega/\langle\Omega\rangle$ on σ (with the exception of one value of $d_c = 4a$ in figure 5(b), to be discussed below). The exponent of the resulting power law is found to be 1 within a statistical error of less than 4%. Hence, the relative fluctuations in the coupling strength J increase linearly as a function of the disorder amplitude σ , in the same way as already known for the resonant frequencies [26]. We can thus write

$$\frac{\delta J}{\langle J \rangle} = \alpha\sigma, \quad (3)$$

$$\frac{\delta\Omega}{\langle\Omega\rangle} = \beta\sigma, \quad (4)$$

where α and β depend on the specific molecule configuration. The data in figures 5(a) and (b) clearly indicate that $\delta J/\langle J \rangle$ increases faster than $\delta\Omega/\langle\Omega\rangle$, as σ increases. This leads to the main conclusion of this work, namely, the coupling strength is more sensitive to disorder than the normal mode frequencies. The power laws in equations (3) and (4) are expected to be the same because coupling strengths and resonant frequencies are ultimately affected by the same phenomenon in the presence of disorder, i.e., area fluctuations of the slab holes [30]. However, since the parameters J and Ω are mostly determined by the region between (region with holes) and inside (region with no holes) the cavities, respectively, disorder induced fluctuations are expected to grow faster in the former than in the latter, i.e., $\alpha > \beta$. Moreover, larger values of J —usually obtained at small cavity–cavity separations—are more robust against disorder than the smaller ones. This dependence emerges clearly when relating the normal mode splitting in figures 1(c) and (d), with the factor α obtained from figures 5(a) and (b). It appears clearly that the smaller the normal mode splitting, the larger α . The extreme case with $d_c = 4a$ in the 60° molecule corresponds to a vanishing normal mode splitting, i.e. to a vanishing J . Then, the relative





fluctuations in J eventually become larger than the average value of J , and the dependence on σ is no longer linear.

From the results displayed figure 5, the linear dependence in equation (3) remains undoubtedly valid as long as $\delta J/\langle J\rangle < 0.1$, which is the region where the disorder induced fluctuations in J can be considered as a small effect. This sets an upper bound to the disorder amplitude, given by $\sigma_{\max} = 0.1/\alpha$. For typical photonic molecules as those considered here, this upper bound translates to $\sigma_{\max} \sim 0.02a$, which is safely far from the fabrication accuracy currently achieved in Si and GaAs PhC. For designs with particularly small couplings however, such as in the 60° molecule at $d_c = 4a$, the bound is already reached for $\sigma_{\max} < 0.001a$. This leads to the general conclusion that, when designing a PhC structure with very small couplings, disorder may represent a major obstacle to achieving the nominal values of the coupling in fabricated structures.

4. Conclusions

We have studied the effects of disorder on the coupling strength of coupled PhC cavities, by combining microscopic simulations of the electromagnetic modes with a coupled-mode model. We have found that the relative fluctuations of the coupling strength J and normal modes frequencies Ω increase linearly with the Gaussian disorder amplitude σ . Furthermore, the disorder induced fluctuations $\delta J/\langle J\rangle$ increase faster than $\delta\Omega/\langle\Omega\rangle$ for increasing σ , leading to the conclusion that the so called photon hopping parameter J is more sensitive to random imperfections than the normal modes of the coupled cavity system. This result sets an upper bound to the amount of disorder that can be supported by coupled PhC structures, in order for the nominal coupling to be actually realized in fabricated structures. For most of the configurations studied here, we estimate this bound to lie quite above the current fabrication accuracy achieved in modern fabrication techniques for typical Si and GaAs PhC slabs [19, 46]. A more stringent bound is instead found in cases where the nominal value of J , as predicted by the coupled cavity design, is very small. In these cases, state-of-the-art fabrication may be insufficient to produce structures where the nominal coupling is systematically realized.

The present findings on the statistical distribution of the coupling J are essentially determined by the local disorder properties in the coupling region of the PhC. The present conclusions can then be generalized to other coupled PhC structures, such as coupled cavities with different geometries or cavities coupled to waveguides. They provide general guidelines to estimate the disorder induced statistical fluctuations of the coupling strengths, when designing a coupled PhC structure.

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