Optimizing H1 cavities for the generation of entangled photon pairs

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Abstract. We report on the theoretical investigation of photonic crystal cavities etched on a suspended membrane for the generation of polarization entangled photon pairs using the biexciton cascade in a single quantum dot. The implementation of the spontaneous emission enhancement effect increases the entanglement visibility, while the concomitant preferential funneling of the emission in the cavity mode increases the collection of both entangled photons. We demonstrate and quantify that standard cavity designs present a polarization-dependent emission diagram, detrimental to entanglement. The optimization of H1 cavities allows us to obtain both high collection efficiencies and polarization-independent emission, while keeping the high Purcell factors necessary for high-quality entangled photon sources.

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Deterministic sources of entangled photons are an important asset for future quantum communication networks [1] or quantum information processing algorithms [2, 3]. In the latest experimental demonstrations of the above applications [4]–[8], the entangled photon source is based on parametric downconversion. Such nonlinear sources of entanglement can combine narrow spectral bandwidths with a maximal generation rate [7, 9, 10]. Although these sources may be very useful and easy to implement, they always suffer from the Poissonian statistics of the emitted photon pairs leading to multipair emission and thus decreasing the fidelity of entanglement [11]. It is hence mandatory, for efficient experimental realizations, to develop deterministic sources of entangled photons delivering one and only one photon pair per excitation cycle, while collecting the maximum of the emitted photons. Single quantum dots are an interesting candidate for such realization. The cascaded emission from the biexciton state of a perfect quantum dot leads to the emission of polarization entangled photons [12]. But in real quantum dots, due to the excitonic energy splitting, the emitted photons are not entangled since the decay path can be extracted from the photon’s wavelength. Entanglement can be restored by either spectrally filtering the photon pairs [14], hence reducing the quantum efficiency of the source, or by choosing a quantum dot with null energy splitting [15], which is a time-consuming task. It is also possible to reduce the exciton level splitting with the help of a magnetic [16] or electric field [17], although such techniques change the branching ratio of the decay paths, which reduces the fidelity of entanglement.

Another approach consists of implementing cavity quantum electrodynamics (CQED) effects by embedding a single quantum dot in a microcavity. For example, entangled photon pairs can be obtained by implementing strong coupling between a quantum dot and a photonic crystal microcavity [18] or by implementing weak coupling and taking advantage of the Purcell effect [19]. The latter effect may also be used to enhance the collection efficiency of the emitted photons [20, 21]. One promising microcavity for this purpose is the single defect hole cavity in a triangular lattice of holes (H1) etched on a suspended membrane, due to its small mode volume and its polarization degeneracy. Such cavities have been extensively studied [22, 23] in terms of emission diagram, quality factor and collection efficiency [21, 24]. It has been pointed
out that due to technological imperfections, the two polarization modes are not degenerate in energy, making the cavity unsuitable for the generation of entangled states. However, by proper design of the cavity and atomic force microscope (AFM) oxidation, it is possible to minimize the energy splitting \[25\]. While all these studies add important knowledge on photonic crystal cavities, none of them addresses two of the fundamental issues for the creation of entangled photon pairs, namely the spatial mode distinguishability of the two polarization modes and the loss of entanglement due to the spatial mismatch of the quantum dot with respect to the photonic crystal cavity. In fact, in the first case, the photon’s polarization is correlated with the spatial distribution of the emission pattern, leading to loss of entanglement. In the second case, due to the spatial mismatch, each polarization will undergo a different Purcell effect, hence unbalancing the branching ratio during the biexciton cascade, leading to non-maximally entangled states.

In this paper, we report on the theoretical investigation of H1 photonic crystal cavities etched on a slab membrane, in order to obtain both high collection efficiencies for both photons and a high overlap between the two dipole energy-degenerate modes. The dependency of the Bell inequalities as a function of the mode overlap is derived. We also investigate the impact of the position of the quantum dot inside the cavity on entanglement visibility and collection efficiency. We deduce some technological benchmarks for the practical realization of such a source.

1. Entangled state density matrix for non-overlapping modes

Polarization entangled photon pairs can be obtained if and only if, even in principle, the polarization of the photon cannot be determined by measuring another degree of freedom, for example the photon’s energy. In real quantum dots, the energy splitting of the exciton transition, spin-flip effects and mutual dephasing introduce which-path information destroying the entangled state (see appendix A and figure A.1). Such effects have been theoretically studied, taking into account all, or part, of the dephasing mechanisms \[19, 29, 30\]. In the same way, if the emission modes with horizontal (\(H\)) and vertical (\(V\)) polarization do not perfectly overlap, the fidelity of the entangled state will be reduced. The effect of non-perfect overlap on the density matrix \(\rho\) of the photons pair (equation (A.1)) can be estimated under the assumption that each emitted photon is perfectly coupled in the cavity mode, which we will discuss in the next section.

The cavity mode is doubly degenerated in polarization, due to the \(C_6\) symmetry of the H1 cavity. The possible symmetry breaking of the cavity due to technical imperfections will be briefly discussed in the last section. We can consequently describe the photons polarization in the \((H, V)\) basis defined by the excitonic splitting of the dot, independently of its orientation with regard to the orientation of the photonic crystal. We define \(\Phi_H(\vec{r})\) (respectively, \(\Phi_V(\vec{r})\)) the complex spatial far-field distribution of the horizontal (\(H\)) (respectively, vertical (\(V\))) polarization modes. Propagation occurs along the orthogonal direction to the photonic crystal membrane and \(\vec{r}\) denotes the radial vector perpendicular to the propagation axis. The cavity is positioned at the focal point of a microscope objective, which transforms the emitted far-field into the complex transverse shape of a propagative beam. In the first-order approximation, \(\Phi_H\) and \(\Phi_V\) are real and positive, corresponding to the case where the transverse phase is constant in the propagative modes (plane wave approximation). Let \(t(r)\) be the function describing the active areas of the detectors placed along the propagation axis. There are, in fact, two distinctive
detectors (one for each photon of the pair [19]) but we suppose that they have the same sensitive area for the sake of simplicity. Finally, let \( k \) and \( e \) be

\[
k = \int d^2r \, t(\vec{r}) \Phi_H(\vec{r}) \Phi_V(\vec{r}),
\]

\[
e = \int d^2r \, t(\vec{r}) \Phi_H^2(\vec{r}) = \int d^2r \, t(\vec{r}) \Phi_V^2(\vec{r}).
\]

The overlap factor \( K \) can be expressed as \( K = k^2/e^2 \).

The final expression of the detected photon pair density matrix in the case of non-maximal overlap between the two emission modes is

\[
\rho = \begin{pmatrix}
\alpha & 0 & 0 & (d - ic_1)K \\
0 & \frac{1}{2} - \alpha & c_2 K & 0 \\
0 & c_2 K & \frac{1}{2} - \alpha & 0 \\
(d + ic_1)K & 0 & 0 & \alpha
\end{pmatrix}.
\]

The definitions of the constants \( \alpha, d, c_1 \) and \( c_2 \) used to describe the dot and details on the model used are given in appendices A and B, respectively. Note that only the coherence terms are modified by the overlap factor \( K \). When the two modes do not overlap \( (K = 0) \), the mutual coherence is erased and entanglement vanishes. On the contrary, maximally entangled states can only be obtained for \( K = 1 \). Following [19], Bell inequalities can be rewritten as \( S = 2\sqrt{2}(\alpha + K * (d - c_2)) > 2 \). Note that even in the case of a single dot emitting maximally entangled photons, a minimum overlap of \( K > 2/\sqrt{2} - 1 = 41\% \) is required in order to violate Bell inequalities.

2. About the spectral resonance of the dot lines in the cavity mode

An important feature for the generation of a highly efficient source of entangled photon pairs is related to the collection efficiency of both photons \( \eta_{\text{EPR}} \), defined by \( \eta_{\text{EPR}} = \eta_X * \eta_{XX} \), where \( \eta_X \) and \( \eta_{XX} \) are the collection efficiencies of the exciton and biexciton, respectively. Hence, if only one of the photons is efficiently collected, the overall collection efficiency will be lowered. If the two emission lines are coupled with the same cavity mode, the two individual collection efficiencies depend on the coupling efficiency of both photons in the cavity mode (\( \beta_X \) and \( \beta_{XX} \), respectively) and the collection efficiency \( \eta \) of the mode itself. The fraction \( (1 - \beta) \) of photons not coupled to the cavity mode will most probably not be collected by the microscope objective, since the collection efficiency through a high index material is less than 1% for a single dipole [13]. Therefore, the collection efficiency reads

\[
\eta_{\text{EPR}} = \beta_X * \beta_{XX} * \eta^2.
\]

The fraction of spontaneous emission in the cavity mode, or coupling efficiency, of the biexcitonic transition is \( \beta_{XX} = F_{XX}/(F_{XX} + \gamma_{\text{loss}}) \), where \( F_{XX} \) is its Purcell factor and \( \gamma_{\text{loss}} \) the modification of the spontaneous emission in modes other than the cavity mode. This value is generally close to \( \gamma_{\text{loss}} = 1 \). Hence, a Purcell factor larger than 5 is sufficient to emit more than 80% of the photons in the cavity mode (the same stands for the excitonic transition). Note that for sources based on parametric downconversion, the collection efficiency of each photon is generally limited to 25% [7], except for fibered sources based on four-wave mixing [10].
Figure 1. Red curve: the Purcell factor of the non-resonant biexcitonic line as a function of the Purcell factor on the resonant excitonic line, with $V_{\text{cav}} = 0.7$ and $\delta = 2/900$. Green curve: minimal biexcitonic Purcell factor acceptable for our chosen minimal mode coupling efficiency $\beta_{XX} > 0.8$.

For standard InAs/GaAs quantum dots emitting around $\lambda_{\text{QD}} = 900$ nm, the energy splitting between the two photon lines is around $\lambda_X - \lambda_{XX} = \delta \lambda_X - \lambda_{XX} = 2$ nm [31]. Let us define $\delta = \delta \lambda_X - \lambda_{XX}/\lambda_X$ and consider the exciton in perfect resonance with the cavity mode. The Purcell factor of the biexciton can be written as $F_{XX} = F_X/(1 + 4Q^2\delta^2)$. Considering that $Q = (4\pi^2/3)V_{\text{cav}}F_X$, where $V_{\text{cav}}$ is the cavity volume expressed in $(\lambda/n)^3$ units, we can rewrite the above equation as

$$F_{XX} = \frac{F_X}{1 + \left((8\pi^2/3)V_{\text{cav}}F_X\delta\right)^2}.$$  

(5)

Hence, the Purcell factor of the biexciton rises almost linearly with respect to the Purcell factor of the exciton until $F_{XX} = 12$ equivalent to a quality factor of $Q = 225$. Above this value, increasing the excitonic Purcell factor decreases the biexcitonic Purcell factor due to a too thin mode line (see figure 1). Constraining the biexcitonic mode coupling efficiency $\beta_{XX}$ to be higher than 80%, limits the excitonic Purcell factor between 5 and 120 (for typical values of $V_{\text{cav}} = 0.7$ in the case of H1 cavities). Moreover as demonstrated earlier [19], an excitonic Purcell factor of 10 is sufficient to restore entanglement for a quantum dot with $T_1 = 1/\gamma_1 = 1$ ns, $1/\Gamma_{\text{np}} = 10$ ns and $1/\Gamma = 2$ ns and an energy splitting of less than 5 $\mu$eV. This corresponds to a quality factor of $130 < Q < 1500$. The maximal allowable quality factor corresponds to a line width of 0.6 nm for the cavity mode.

For the rest of the analysis, we consider that the exciton and biexciton photons are emitted in the same cavity mode: the cavity mode is resonant with the excitonic transition, quasi-resonant with the biexcitonic one and degenerate in polarization.

3. H1 cavity for maximally entangled photons

We consider the H1 cavity as a potential candidate for the generation of entangled photon pairs since it sustains two energy degenerate dipole modes with a field maximum in the center of
the cavity. This cavity offers both a low mode volume and theoretically high-quality factors by fine-tuning the inner holes [23]. We are interested in the dipole mode of such a cavity for the following reason. For the generation of entangled photon pairs, both polarizations shall undergo the same effects, same emission diagram, same Purcell factor. While the hexapole mode has been studied for its highly directive emission diagram [26], all modes, other than the dipole mode, present a node in the center of the cavity. The quantum dot should hence be placed out of the center of the cavity, breaking the $C_6$ symmetry as will be discussed in the following section.

Simulations on H1 cavities were performed with a 3D finite-difference time-domain (FDTD) method, using a freely available software package with subpixel smoothing for increased accuracy [27]. The simulated structure is depicted in figure 2. The H1 photonic crystal (figure 2(a)) has a lattice constant equal to $a = 270$ nm and the holes have a radius of $r_h = 80$ nm. The refractive index of the GaAs membrane is equal to $n = 3.46$. Above and below the membrane, a free space volume is inserted, with a thickness of $3a$. With the above parameters, the emission wavelength of the H1 cavity is centered around 950 nm, which is the wavelength of InAs/GaAs quantum dots. The simulation volume is finally surrounded by split field perfect matched layers (PML). A temporally short Gaussian dipole pulse (with a width of 10 optical oscillations) is launched in the center of the cavity (figure 2(b)) and used as a white light source. After extinction of the source, the electromagnetic field evolves freely over a time corresponding to approximately 300 optical cycles of the source, after which all low-quality factor modes have radiated, thus leaving only the desired cavity mode in the simulation volume. In such conditions, the decay of the field amplitude at some fixed non-nodal point inside the cavity follows a simple exponential function with a rate $\Gamma_c$. The emission wavelength is determined by measuring the optical oscillation frequency.

The collection efficiency is defined as the ratio between the incident power within a given emission cone normal to the membrane, over the total emitted power. This corresponds to the collection efficiency of either the exciton $\eta_X$ or the biexciton $\eta_{XX}$, but does not take into account the probability of emitting the photon in the cavity mode. At any given time, the total emitted power is given by $P_{\text{ref}} = \Gamma' W$, where $W$ denotes the energy inside the cavity, and $\Gamma'$ is the intensity decay rate ($\Gamma' = 2\Gamma_c$). Let $U$ be the total energy in the simulated volume at time $t$. 

Figure 2. H1 photonic crystal cavity. The inner holes are shifted by the quantity $d$ from 0 (standard H1 design) to $0.18a$. The blue line is the plane, where the field is registered at the end of the simulation for radiative pattern calculations.
Figure 3. Emission patterns for various hole displacement $d$ for a membrane thickness of $h = 0.14 \, \mu m$. Each pattern is normalized to its maximum value. The distance to the center is $\sin(\theta)$, where $\theta$ is the normal angle to the membrane. The gray (respectively, black) circle represents an objective of numerical aperture (NA) = 0.5 (respectively, NA = $\sin(\pi/4)$ = 0.7).

The energy outside the cavity ($U_{\text{out}}$) corresponds to the energy emitted by the cavity which has not yet reached the edge of the simulation volume, $U_{\text{out}} = \Gamma' \ast W' \ast D / c$ with $D$ being the radius of the simulated volume and $c$ the speed of light. Thus $U = W \ast (1 + D / c)$. Since $D$ is only a few micrometers wide, $D / c \ll 1$, and the total emitted power can be written as $P_{\text{ref}} = 2\Gamma_c U$.

The emission mode of the cavity is estimated following [28] (mainly equation (23)). This method relies on the complex value of the electromagnetic field on a plane ($P$) just above the membrane (see figure 2(b)) at some time (in our case the end of the simulation). The real part of the electromagnetic field is directly measured on ($P$), and the imaginary part is deduced from measurements of the real part of the electromagnetic field a quarter oscillation later (at the cavity’s resonant frequency), taking into account the losses induced during this quarter of cycle. This allows us to extract the far-field emission mode from the light-cone of the spatial Fourier transform of the field with a unique simulation run in real values, thus saving valuable calculation time. Emission patterns for a membrane thickness of $h = 0.14 \, \mu m$ as a function of the hole displacement $d$ are depicted in figure 3 and correspond qualitatively to the emission patterns calculated by Roemer et al [23] using a 3D finite element Maxwell solver. For small hole displacements ($d \lesssim 0.10$), the emission diagram is almost spherical. By increasing the hole displacement ($d \geq 0.14$), a pronounced, directional Gaussian-like, central peak appears, but this pattern vanishes for strong hole displacement ($d \geq 0.26$).

A systematic analysis of the quality factor ($Q$), the single photon collection efficiency ($\eta$) and the mode overlap ($K$) has been performed by varying two parameters: the hole displacement $d$ and the membrane thickness $h$. Figure 4 summarizes the results obtained on the mode overlap and on the collection efficiency estimated for light collection through a microscope objective with an NA of 0.5. A more detailed view of the variation of these parameters as a function of the hole displacement is given in figure 5, in which the membrane thickness is fixed to $h = 0.14 \, \mu m$ and three objective NAs have been taken into account (0.2, 0.5 and 0.7). The resonance
Figure 4. Quality factor, collection efficiency and mode overlap as a function of the hole displacement ($d$, in crystal units $a$) and membrane thickness ($h$, in $\mu m$). The shaded regions are the parameter’s domain of value, where the H1 cavity does not sustain a dipole mode. The black line on the quality factor mapping defines the limit $Q = 1500$.

Figure 5. Quality factor, collection efficiency and mode overlap as a function of the hole displacement ($d$, in crystal units $a$) for a membrane thickness $h = 0.14 \mu m$. The collection efficiency and the mode overlap are calculated for $NA = 0.2$ (red curves), $NA = 0.5$ (blue curves) and $NA = 0.7$ (green curves).

Wavelength $\lambda_c$ of the cavity depends strongly on both parameters $d$ and $h$. For the more studied membrane thickness $h = 0.14 \mu m$, a good approximation is $\lambda_c = 903 + 693d - 1.66d^2$ (expressed in nm) with a maximal deviation of 1 nm. A global homothetic transformation of the design, including the membrane thickness, should be applied to tune the cavity to the desired wavelength but is not taken into account here. The modal volume varies as $V_{\text{cav}} = 0.69 - 3.13d + 24.5d^2$ with a maximal deviation below 0.01 for this membrane thickness.

The limitations of the $Q$ factor determined in the previous part of this paper are satisfied (figure 4) for small hole displacement ($d \leq 0.08$) or a high one ($d \geq 0.2$). However, high emission mode overlap and high collection efficiency are also necessary. From figure 4, we observe that the highest collection efficiencies are obtained for a membrane thickness of $h = 0.14 \mu m$. A cross section of figure 4 is represented in figure 5. Clearly, for a small hole displacement ($d \leq 0.09a$) the mode overlap is almost unity (in excess of 95%), but at the expense of a low collection efficiency, below 15% for standard microscope objective, and does not exceed 30% for $NA = 0.7$. Note that the theoretical limit for each photon is 50% since light
is emitted upwards and downwards with the same probability. The adjunction of a mirror on one of the sides of the suspended membrane would increase the overall collection as pointed out in [26]. The emission diagram (figure 3) for a hole displacement of \( d = 0.09a \) clearly explains the situation. The mode is almost uniform in every direction, giving rise to a high mode overlap, and the collection efficiency scales as the objective NA. Consequently, even if most of the signal escapes from the cavity, the uniform emission diagram prohibits an efficient coupling of the photons in an optical fiber.

In the range \( 0.11a \leq d \leq 0.15a \) the mode overlap presents a distinct dip down to 40% for an objective with \( \text{NA} = 0.7 \), which is the minimum allowable for perfect dot to emit entangled photon pairs (see section 1). The collection efficiency drops to the same extent. In this region, the quality factor reaches its maximum \( (d = 0.14a) \). This drop in the collection efficiency corresponds to better confinement of the light inside the photonic crystal slab and a reduction of vertical losses at the \( \Gamma \) point as one would expect.

For even larger hole displacements \( (0.15 \leq d \leq 0.25a) \) the single photon collection efficiency increases sharply reaching 25% for an \( \text{NA} = 0.5 \) (and \( d = 0.18a \)), corresponding to a twofold increase compared with standard H1 cavity. At the same time, the mode overlap increases up to 95% reaching almost the values obtained at low values of \( d \). The mode profile (figure 3) is almost \( \text{TE}_{00} \) in the propagation direction perpendicular to the membrane. Using an objective with \( \text{NA} = 0.2 \) increases the overlap up to almost 100% but at the expense of a low collection efficiency. On the other hand, \( \text{NA} = 0.7 \) increases the collection efficiency by a factor of 1.5 compared with \( \text{NA} = 0.5 \), but the mode overlap does not exceed 83% indicating that almost half of the energy is astigmatic.

In order to satisfy the above condition on the quality factor, the best compromise with high collection efficiency and high mode overlap, a hole displacement of \( d = 0.22a \) and membrane thickness \( h = 0.49\lambda_c/n \), with an objective with \( \text{NA} = 0.5 \), seems to be the optimum in terms of modal collection efficiency (of the order of 23% with a maximal calculated value of 50%) and mode overlap (of the order of 96%), while keeping the quality factor at a reasonable value \( (Q = 1100) \).

Further increase of the collection efficiency can be obtained by adding a Bragg mirror below the membrane, at adequate distance \([26]\) so as to create a constructive interference between the light emitted upwards and the downwards emitted reflected light. The emission diagram due to the presence of a Bragg mirror will not be modified leading to a total collection efficiency per photon of 44%. Considering that the exciton line is in perfect resonance with the cavity and has a Purcell factor of 20, and that the biexciton undergoes a Purcell factor of 5, the overall collection efficiency of the entangled pair will be \( \eta_{\text{EPR}} = 44\%^2 \times 0.95 \times 0.8 = 15\% \), which is two times greater than the collection efficiency one can obtain from parametric downconversion \( (25\%^2 = 6\%) \).

4. Impact of the position of the dot in the cavity

Until now the quantum dot has been considered to be perfectly placed in the center of the cavity, implying that both polarizations undergo the same Purcell effect and that the cavity mode is equally fed for both polarizations. Deterministically aligning a photonic crystal around a single quantum dot so that the dot is positioned in the center of the cavity is technologically challenging but mandatory. Several techniques are being developed \([32, 33]\), although due to experimental uncertainties (which are essentially due to the electronic beam lithography
process), the mismatch of the quantum dot position with respect to the center of the H1 cavity can be up to 10 nm [32]. While an energy split photonic crystal cavity mode is as detrimental to entanglement as the spatial position mismatch, it is possible to correct the technology-induced mode degeneracy by local AFM oxidation [25]. We shall restrain the rest of the discussion to the case of spatially misplaced quantum dots, since our analysis places a new benchmark on the quantum dot positioning.

The position mismatch implies a breaking of the $C_6$ symmetry. The position of the dot will be identified by a direction $X$, as shown in figure 6(a), the $Y$-direction being orthogonal to the $X$-direction. The two polarization modes of the cavity remain unchanged. Therefore, the sustained modes of the cavity will be described in the basis $(X, Y)$ and no longer in the $(H, V)$ basis. Due to the mismatch with the cavity modes, the dipole will preferentially excite one of the modes ($X$ or $Y$ polarized) leading to an unbalance of the fraction $\beta_i$ ($i \in \{X, Y\}$) of spontaneous emission in the cavity mode. Inevitably, this will in turn impact the entanglement visibility. Note that it only affects the unbalance of the spontaneous emission and not the emission diagram of the cavity mode, which remains completely unaffected.

Figure 6(b) depicts the normalized $\beta_i$ factor as a function of the position mismatch along the $X$-direction for both polarizations. The curves are normalized with respect to the case with null mismatch. The $\beta_i$ factor is then deduced from the amplitude ratio between the electrical field at the position $X, Y$ with respect to the maximum of the field. The effect of an asymmetric Purcell factor on Bell’s inequality is modeled in appendix C of this paper.

We define the adimensional ratio $r = T_1^{\text{bulk}} \delta \omega / (\hbar F_p^{\text{max}})$ where $T_1^{\text{bulk}}$ is the bulk lifetime of the dot, $2\hbar \delta \omega$ the excitonic energy splitting and $F_p^{\text{max}}$ the maximal Purcell effect of the cavity (at zero spatial mismatch). For any experimental values of $T_1^{\text{bulk}}$, $2\hbar \delta \omega$ and $F_p^{\text{exp}}$, we estimate an $r$ value and report it on the $y$-axis of figure 6(c). In the same figure is plotted the maximum tolerable figure of merit $r$ to obtain at least a Clauser–Horne–Shimony–Holt (CHSH) inequality of $S$, as a function of the quantum dot displacement (calculated using the formalism introduced in appendix C). Entanglement fidelity increases when $r$ tends to zero. For example, in the case of a centered dot with an excitonic bulk lifetime of 1 ns, an excitonic energy splitting of about 2 $\mu$eV, submitted to a maximal Purcell factor of 10 and not subjected to incoherent
processes, the figure of merit \( r = 0.3 \) allows \( S \) to reach a value above 2.6. Conversely, Bell’s inequality is hardly violated \( (S = 2) \) if the same dot is about 70 nm away from the center of the cavity. For a more usual value of the excitonic splitting \( (5 \mu \text{eV}) \), the maximal spatial mismatch enabling for Bell’s inequality violation drops to 10 nm. A figure of merit \( r \), violating the Bell inequalities \( (\text{CHSH} > 2) \), cannot always be defined as a function of the spatial mismatch. For such displacement values, Bell inequalities are not violated even for perfect quantum dots.

One can hence establish a real world technological benchmark on the spatial mismatch between the quantum dot and the cavity mode as a function of the excitonic fine structure splitting (FSS). High spatial mismatch can be tolerated in the case of FSS of less than \( \delta \omega \ll 5 \mu \text{eV} \), but becomes critical if the FSS is not reduced to the smallest possible value.

5. Conclusion

In this paper, we address two issues for the realization of an efficient source of entangled photons based on single quantum dots embedded in a photonic crystal cavity. On the one hand, the non-overlapping emission diagram of H1 cavities adds photon path distinguishability, leading to a reduced fidelity of the entangled state. We demonstrate that by properly adjusting the membrane thickness and hole displacement in a modified H1 cavity, it is possible to obtain almost perfect mode overlap while keeping adequate quality factors and maximizing the collection efficiency. On the other hand, spatial mismatch between the quantum dot and the cavity mode rapidly degrades the quantum state. We introduce a benchmark figure of merit giving the required precision on the technological steps in order to obtain high-quality sources.

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Appendix A. Density matrix for a biexciton cascade emission

The density matrix for the cascade emission from the biexciton level has been introduced elsewhere [19]. For the sake of clarity, we report on the main result of the paper.

Considering the biexciton cascade depicted in figure A.1, we define the eigenbasis of the dot involving four levels as follows: \( |2\rangle \) (biexcitonic level), \( |1_H\rangle \) and \( |1_V\rangle \) (two excitonic levels with opposite angular momenta) and \( |0\rangle \) (fundamental level). In this eigenbasis, the emitted photons are linearly polarized along the horizontal \( (H) \) or vertical \( (V) \) directions. The density matrix of the photon pair in this particular basis \( B = \{ H_1H_2, H_1V_2, V_1H_2, V_1V_2 \} \), where the subscript \( i = 1, 2 \) is related to the photon emitted by the biexcitonic and excitonic level, respectively, can be written in the form

\[
\rho = \begin{pmatrix}
\alpha & 0 & 0 & d - ic_1 \\
0 & \frac{1}{2} - \alpha & c_2 & 0 \\
0 & c_2 & \frac{1}{2} - \alpha & 0 \\
d + ic_1 & 0 & 0 & \alpha
\end{pmatrix},
\]

(A.1)
Figure A.1. Schematic description of the two-photon cascade in a typical quantum dot four-level system with an energy splitting $2\hbar \delta \omega$ of the relay level, yielding two collinearly polarized photons (either $H$ or $V$).

where

\begin{align*}
\alpha & = \frac{1}{2} \frac{\gamma_1 + \Gamma_{\text{flip}}}{\gamma_1 + 2 \Gamma_{\text{flip}}} \\
d & = \frac{1}{2} \frac{\gamma_1 (\gamma_1 + 2 \Gamma + \Gamma_{\text{flip}})}{(2 \delta \omega)^2 + (\gamma_1 + \Gamma_{\text{flip}} + \Gamma)^2 - (\delta \Gamma_{\text{flip}})^2} \\
c_1 & = \frac{1}{2} \frac{\gamma_1 \delta \omega}{(2 \delta \omega)^2 + (\gamma_1 + \Gamma_{\text{flip}} + \Gamma)^2 - (\delta \Gamma_{\text{flip}})^2} \\
c_2 & = \frac{1}{2} \frac{\gamma_1 \delta \Gamma_{\text{flip}}}{(2 \delta \omega)^2 + (\gamma_1 + \Gamma_{\text{flip}} + \Gamma)^2 - (\delta \Gamma_{\text{flip}})^2},
\end{align*}

with $\gamma_1$ the exciton decay rate. $\Gamma = \Gamma_H + \Gamma_V$ is the cross-dephasing rate between the two excitonic states. $\Gamma_{\text{flip}} \pm \delta \Gamma_{\text{flip}}$ describe phenomenologically relaxation mechanisms between the two excitation states, leading to incoherent population transfers between these two states ($\delta \Gamma_{\text{flip}}$ takes into account the possible rate asymmetry in this process). $\delta \omega$ is the energy splitting of the excitonic levels. $\Gamma_1$ is the pure dephasing rate induced by dephasing processes that occur simultaneously and attach the same information to the phase and energy of these two excitonic levels. $\Gamma_H$ and $\Gamma_V$ are polarization-dependent pure dephasing rates induced by dephasing processes that do not identically affect the two relay levels and whose impact depends on the polarization of the excitonic states.

Appendix B. Effect of a non-maximal mode overlap on the photon pair density matrix

If we take into account the transversal distribution of the far-field wavefunctions $\Phi_H$ and $\Phi_V$ of the two polarized modes $H$ and $V$ of the cavity, the density matrix expressed in appendix A...
The matrix of the photon pair in the polarization basis is
\[ \rho(\vec{r}_1, \vec{r}_2)_{xy,uv} = \Phi_x(\vec{r}_1) \dagger \Phi_y(\vec{r}_2) \dagger \Phi_{uv}(\vec{r}_1) \Phi_{uv}(\vec{r}_2), \]  
(B.1)

with \( xy \) and \( uv \) \( \in \mathcal{B} \) and \( \rho_{xy,uv} \) being the density matrix element on line \( xy \) and column \( uv \). \( \rho(\vec{r}_1, \vec{r}_2)_{xy,uv} \) is the density matrix element on line \( xy \) and column \( uv \) of the new density matrix \( \rho(\vec{r}_1, \vec{r}_2) \). \( \vec{r}_1 \) and \( \vec{r}_2 \) are the transversal position of the excitonic and biexcitonic photons.

With \( t(\vec{r}) \) being the detector sensitivity defined in the first part of the paper, the density matrix can be reduced for the detected photon pairs to
\[ \rho = \frac{\int d^2r_1 \int d^2r_2 \ t(\vec{r}_1) t(\vec{r}_2) \rho(\vec{r}_1, \vec{r}_2)}{\text{Tr} \left( \int d^2r_1 \int d^2r_2 \ t(\vec{r}_1) t(\vec{r}_2) \rho(\vec{r}_1, \vec{r}_2) \right)}, \]  
(B.2)

which leads to equation (3).

**Appendix C. Effect of an asymmetry in the Purcell effect**

Independent of the work in the two previous appendices, the asymmetric branching ratio induced by a polarization-dependent Purcell factor can be modeled as follows. Let the state of the system (dot and optical fields) be
\[ |\Psi(t)\rangle = p_2(t)|2; \emptyset; \emptyset\rangle + \sum_{u=H,V} \int d\omega_2 p_u(\omega_2, t)|1_u; \vec{u}, \omega_2; \emptyset\rangle \]
\[ + \sum_{u=H,V} \int d\omega_2 d\omega_1 p_{uu}(\omega_1, \omega_2, t)|0; \vec{u}, \omega_2; \vec{u}, \omega_1\rangle, \]  
(C.1)

where the first of the three entries within the ket refers to the quantum dot’s level, the other two entries refer to the first and second emitted photons of polarization \( \vec{u} \) and pulsation \( \omega_i \) \( (i = 1, 2, \) respectively). (See figure A.1. We distinguish here the emission rates \( \gamma_1 \) and \( \gamma_2 \) with respect to both polarizations \( H \) and \( V \). We assume that incoherent processes are negligible, so that crossed terms combining horizontal and vertical orientations disappear.)

The expressions of the \( p_2, p_u \) and \( p_{uu} \) coefficients are determined using the Wigner–Weisskopf approximation. Considering the system at long times \( (t \gg 1/\gamma_1 \) and \( \gamma_2 \) the terms \( p_2(t) \) and \( p_u(\omega_2, t) \) tend to zero, which gives a state that can be factorized into a radiative part \( |\Psi_k\rangle \) and the fundamental source state \( |0\rangle \). Considering no spectral filtering, the density matrix of the photon pair in the polarization basis is
\[ \rho = \int d\omega_1 d\omega_2 |\omega_2, \omega_1| |\Psi_k\rangle \langle \Psi_k| |\omega_2, \omega_1\rangle, \]  
(C.2)

\[ = \sum_{u,v=H,V} |\vec{u}\vec{v}\rangle \langle \vec{v}\vec{u}| \int d\omega_2 d\omega_1 p_{uv}(\omega_1, \omega_2, \infty) p_{vv}(\omega_1, \omega_2, \infty)^*, \]  
(C.3)

\[ = \frac{1}{2(1 + 2\delta F^2)} \begin{pmatrix}
(\delta F + 1)^3 & 0 & 0 & (1 - \delta F^2)^2 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
(1 - \delta F^2)^2 & 0 & 0 & (\delta F - 1)^3 \\
\end{pmatrix}, \]  
(C.4)
where we defined the relative difference of Purcell factors \( \delta F = (F_H - F_V)/(F_H + F_V) \) and the normalized splitting \( g = 2\delta \omega/(\gamma_1\text{bulk}(F_H + F_V)) \). \( \delta F \) is approximated from the ratio between the modal coupling factors as: \( (\beta_H - \beta_V)/\gamma_H(\gamma_H + \gamma_V) \). In the same way as in [19], we deduce the expression \( S \) of the Bell test, from which we deduce data presented in figure 6(c).

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