Computation and optimization of the Purcell factor of an open tunable Fabry-Pérot microcavity

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Abstract

The spontaneous emission of atoms can be controlled by placing them between two mirrors that form an optical cavity [1]. Rapid advances in material processing techniques in the last 10 years have made it possible to fabricate microscopic optical cavities that can be finely tuned into resonance with the emitter [2]. This has enabled progress in single-photon sources, nano-lasers and spectroscopy of new nano-emitters such as semiconductor quantum dots and Nitrogen-vacancy centres in diamond. Here we introduce a step-by-step method for computing the Purcell factor of the latest generation of open tunable Fabry-Pérot microcavities used in micro-photoluminescence studies. We discuss how the Purcell factor can be optimised as a function of the cavity’s geometry and find the conditions for resonance with the emitter. Subtleties such as the optical properties of the emitter and penetration depth of the electric field into the cavity mirrors are also considered.

I. INTRODUCTION

If a two-level emitter such as an atom in free space is initially in an excited state, the probability of remaining in the excited state decreases exponentially due to spontaneous emission.

\[ P_{ex} = e^{-\gamma t}. \] (1)

Spontaneous emission arises from the coupling between the electric dipole of the emitter and vacuum states. The rate of decay can be modified by confining the emitter inside an optical microcavity [1, 3, 4], resulting in an experimentally measurable change of the lifetime of the emitter’s excited state. This is known as the Purcell effect [5], quantified by a dimensionless factor

\[ F_P \equiv \frac{\gamma_{\text{cav}}}{\gamma}. \] (2)

called the Purcell factor, where \( \gamma_{\text{cav}} \) is the decay rate in the cavity.

The Purcell effect occurs because the cavity changes the density of modes that the emitter can decay into. Assuming that the wavelength of the emitter’s spectral line matches that of the cavity’s optical mode, such that the two are resonant, the Purcell factor is expressed as

\[ F_P = \frac{3}{4\pi^2} \frac{\lambda^3}{Q_{\text{eff}}} \] (3)

where \( V \) is the volume of the mode occupied by the electric field [6–8], and \( Q_{\text{eff}} \) is the effective quality factor of the cavity-emitter system, \( Q_{\text{eff}} = (Q_{\text{cav}}^{-1} + Q_{\text{em}}^{-1})^{-1} \). We will concern ourselves
only with the quality factor of the cavity, $Q_{\text{cav}}$, and assume that the emitter’s quality factor, $Q_{\text{em}}$, is a fixed intrinsic quantity.

The coupling between the emitter and the cavity mode can be described by the Jaynes–Cummings model [9]. The strength of coupling is characterized by a coupling constant, defined as

$$g_0 = \left( \frac{\mu_{12} \omega_0}{2 \varepsilon_0 \hbar V} \right)^{1/2}$$

where $\omega_0$ is the atomic transition angular frequency (equal to the angular frequency of the cavity mode) and $\mu_{12}$ is the matrix element of the electric dipole transition. We note that the coupling constant has dimensions of frequency $s^{-1}$. Comparing it to the decay rate of the emitter in free space, $\gamma$, and that of the cavity, $\kappa$, we can distinguish two regimes. When $g_0 \gg \kappa, \gamma$, we enter the so-called strong-coupling regime where the coupling rate dominates the loss rate, leading to a coherent and reversible exchange of energy between the emitter and cavity mode. Photons emitted into the cavity mode undergo cycles of re-absorption by the emitter and re-emission as they are less likely to leave the cavity. This regime has applications in quantum information processing since it allows us to manipulate the quantum state of the emitter [10, 11]. However, the experimental challenges to fabricate very high-quality optical microcavities required to operate in this regime can be significant.

When $\kappa, \gamma \gg g_0$, the loss rate exceeds the cavity coupling rate. Once generated, the photon leaks out of the cavity faster than it can be re-absorbed by the emitter. This is called the weak-coupling regime where spontaneous emission of the emitter is modified by the cavity in such a way that emission into the cavity mode is favoured. This is in huge comparison with the original arbitrary direction of emission when the emitter is in free space. Such a feature can be used to build bright single-photon sources which is fundamental for technological applications in photonics such as distributed quantum networks [12] or quantum cryptography [13–15].

Since the first experimental demonstration of Purcell-factor cavity-enhanced spontaneous emission from single-atom in the 1980s [16] and those from semiconductor quantum dots in the 2000s [17, 18], significant advances have been made in engineering microcavities. A promising type of optical cavities are open and tunable hemispherical microcavities [2]. They allow experimentalists to insert emitters into the cavity and to tune its optical mode into resonance with the emitter and to optimise positioning with piezo-electric actuators.

Notice that the Purcell effect does not guarantee that the decay rate of the emitter is increased. In fact, both cavity-enhanced and inhibited emission have been observed in experiments [19, 20]. In order to reach Purcell enhancement of the emission, we should make
sure that the emitter resonates with the cavity, where geometrical parameters of the cavity are crucial. Therefore, in this article, we will compute the Purcell factor as a function of the geometric parameters of hemispherical cavity and find the highest possible value of $F_P$ to maximise the brightness of a given emitter.

The cavity we study consists of a flat mirror and a spherical concave mirror facing towards each other. Each mirror is a Distributed Bragg Reflector [21] with high reflectivity. Our nominal emitter is a semiconductor quantum dot (QD), assumed to be a point-source, with central wavelength $\lambda_0 = 537$ nm and linewidth 2.5 nm. The QD is deposited on the flat mirror and is positioned on the longitudinal optical axis of the cavity.

II. REFLECTIVITY OF THE BRAGG MIRROR

A. Introduction to Bragg Mirror

The Distributed Bragg Reflector (DBR, or Bragg mirror) is a key structural component of our microcavity that determines its internal reflectivity.

A Bragg mirror consists of alternate layers of two dielectric materials with different refractive indices, $n_1$ and $n_2$. A layer with refractive index $n$ has thickness $d = \lambda_0/4n$, where $\lambda_0$ is the central wavelength. We denote the number of layer pairs of the two materials as $N$, so that there are $2N$ individual layers in total. In our cavities, the Bragg mirrors comprise 8 and 16 layer pairs on the spherical and flat sides respectively. The imbalanced reflectivities ensure that light can emerge from the cavity from the spherical side (with lower overall reflectivity) where an objective lens can be placed to collect the light.

The flat Bragg mirror is manufactured by coating these alternate layers of material onto a substrate. Whereas for the spherical mirror, a spherical hole is created on the substrate before coating.

B. Theoretical Analysis

Figure 1 shows a schematic of a Bragg mirror with a plane wave incident from the left hand side. We assume that the Bragg mirror is wide enough in the transverse direction so that diffraction losses can be neglected. When the incident wave with wavelength $\lambda$ enters the Bragg stack, it will split into waves travelling forwards and backwards at the interface.
between each layer due to reflection and transmission. The electric field must satisfy the wave equation

$$\frac{\partial^2 E}{\partial t^2} - \frac{c^2}{n^2} \frac{\partial^2 E}{\partial x^2} = 0$$

(5)

where $x$ is the coordinate along the direction of propagation, $c$ is the speed of light in vacuum and $n$ is the refractive index.

For a component of a given angular frequency, $\omega$, the general solution to Eq. (5) is

$$E(x,t) = \mathcal{E}(x) e^{-i\omega t}$$

(6)

$$\mathcal{E}(x) = Ae^{ikx} + Be^{-ikx} \quad A, B \in \mathbb{C}$$

(7)

where $\mathcal{E}(x)$ is the spatial part of the wave and $k = 2n\pi/\lambda$ is the wave vector.

In Figure 1 the parameters $a_j, b_j$ and $t$ are complex amplitudes. The form of electric field across the whole region is

$$\mathcal{E} = \begin{cases} 
    a_0 e^{ik_0 x} + b_0 e^{-ik_0 x} & x < 0; \\
    a_j e^{i n_j x} + b_j e^{-i n_j x} & 0 < x_j < \lambda/4n_j; \\
    te^{ik_0 x_{2N+1}} & x_{2N+1} > 0.
\end{cases}$$

(8)

where $k_0 = 2\pi/\lambda$ is the wave vector in vacuum, $n_j$ and $d_j = \lambda_0/4n_j$ are the refractive index and thickness of the $j$th layer respectively and $x_j$ is the distance to the left side of the $j$th layer with the $(2N + 1)$th layer being the air gap on the right.

![Diagram](image.png)

FIG. 1. Structure of the Bragg mirror and the waves propagating inside the stack. Light is incident from the left. Parameters $a_j, b_j$ ($0 \leq j \leq 2N$) and $t$ denote the complex amplitudes of waves in each layer. The arrows indicate the directions of propagation. $n_1$ and $n_2$ are refractive indices of each layer.

The complex reflectivity is defined as

$$\tilde{r} \equiv \frac{b_0}{a_0}$$

(9)
Its modulus is the amplitude reflectivity

\[ r \equiv \left| \frac{b_0}{a_0} \right|. \tag{10} \]

And the intensity reflectivity is its modulus squared

\[ R \equiv |\tilde{r}|^2 = r^2. \tag{11} \]

To solve for the reflectivity, we use the condition that the electric field and its first derivative with respect to \( x \) should be continuous at the boundaries. Otherwise the second order derivative of the electric field with respect to \( x \) will diverge and Eq. (5) cannot not be satisfied.

\[
\begin{align*}
\mathcal{E}(x_j = d_j) &= \mathcal{E}(x_{j+1} = 0) \\
\frac{d\mathcal{E}}{dx_j}(x_j = d_j) &= \frac{d\mathcal{E}}{dx_{j+1}}(x_{j+1} = 0)
\end{align*}
\tag{12}
\]

Written in terms of complex amplitudes, we have

\[
\begin{bmatrix}
a_j \\
b_j
\end{bmatrix} = T
\begin{bmatrix}
a_{j+1} \\
b_{j+1}
\end{bmatrix}
\tag{13}
\]

where

\[
T = \begin{bmatrix}
1 + \frac{n_{j+1}}{n_j}e^{-i\phi_j} & 1 - \frac{n_{j+1}}{n_j}e^{-i\phi_j} \\
1 - \frac{n_{j+1}}{n_j}e^{i\phi_j} & 1 + \frac{n_{j+1}}{n_j}e^{i\phi_j}
\end{bmatrix}
\tag{14}
\]

is the transfer matrix and

\[
\phi_j = \begin{cases}
0 & j = 0; \\
k_0n_jd_j = (\lambda/\lambda_0)(\pi/2) & \text{otherwise.}
\end{cases}
\tag{15}
\]

Eq. (13) can also describe the rightmost interface between the \((2N)\)th layer and air by setting \(a_{2N+1} = t, b_{2N+1} = 0\) and \(n_{2N+1} = 1\). In this way, complex amplitudes in the previous layer can be calculated from those in the next layer. Hence we can first express \(a_{2N}, b_{2N}\) in terms of \(t\), then \(a_{2N-1}, b_{2N-1}\) in terms of \(t\), \(\ldots\) all the way to \(a_0, b_0\). Thus the complex reflectivity \(\tilde{r}\) can be determined from Eq. (9) where the factor \(t\) cancels out.

Apart from deriving the transfer relation Eq. (13) from Eqs. (12), one can also start by using the condition that the tangential components of electric field \(\mathbf{E}\) and magnetic field \(\mathbf{H}\) should be continuous at boundaries [22, § 9.7.1]. Using the relation between \(\mathbf{E}\) and \(\mathbf{H}\) in
the electromagnetic wave, this alternative method will arrive at the same transfer relation of complex amplitudes of electric field.

We note that the reflectivity of the Bragg mirror for light of the design wavelength $\lambda_0$ is independent of $\lambda_0$. This is because when $\lambda = \lambda_0$, $\lambda_0$ does not appear in the transfer relation Eq. (13), so the reflectivity is only a function of $n_1$, $n_2$ and $N$.

C. Results of the Bragg Mirror Reflectivity Simulation

Our simulation considers two different layer combinations. One consists of alternate layers of SiO$_2$ and Ta$_2$O$_5$, with $n_1 = 1.4605$ and $n_2 = 2.1453$ or vice versa. The other is SiO$_2$ and TiO$_2$ with $n_1 = 1.4605$ and $n_2 = 2.6620$ or vice versa. A subtlety worth considering is whether the first layer of the DBR should have a lower or higher refractive index, corresponding to $n_1 < n_2$ and $n_1 > n_2$ respectively. As we will see below, this will affect the mode volume of the cavity mode.

Figure 2 illustrates the relationship between the reflectivity of the Bragg mirror and the wavelength for our two media combinations and layer pairs $N = 8$ or 16. For both types of media, the reflectivity profile has a plateau (called the stopband) around the central design wavelength, where reflectivity is near-unity. Notice that the stopband is wider for SiO$_2$ + TiO$_2$. Figure 3 shows the increase in reflectivity of the DBR as the number of layer pairs $N$ increases. We note that the reflectivity at the design wavelength depends only on $n_1$, $n_2$ and $N$. So the dependence of $R$ on $N$ is independent of the choice of design wavelength. As $N$ increases, the reflectivity approaches 100% rapidly.

Comparing Figure 2(a) and (b), it would appear that the SiO$_2$ + TiO$_2$ combination offers near unity reflectivity over a wider wavelength range. In practice, however, this advantage is lost to the SiO$_2$ + Ta$_2$O$_5$ combinations where scattering losses tend to be lower owing to lower surface roughness on mirror coatings, since Ta$_2$O$_5$ is easier to coat.

Table I summarizes the modulus and argument of the complex reflectivities at the central wavelength of the Bragg mirrors, with Ta$_2$O$_5$ being the higher refractive index layer. Bragg mirrors where the first layer has a lower refractive index will not impart a phase shift to the reflected wave, whereas those starting with a higher refractive index layer will result in a $\pi$ phase shift.
FIG. 2. Reflectivity of the Bragg mirrors as a function of the wavelength contrasting stacks with $N = 8$ and $N = 16$ for (a) SiO$_2$ + Ta$_2$O$_5$ and (b) SiO$_2$ + TiO$_2$ combinations. The Bragg mirrors have near-unity reflectivities over a certain range around the central wavelength, $\lambda/\lambda_0 = 1$ and suppress modes outside this range.

FIG. 3. The reflectivity of the Bragg mirror at central wavelength increases rapidly with the number of layer pairs, $N$.

III. MODELLING THE MICROCAVITY

A. Geometry of the Microcavity

Figure 4 shows a cross-section through the microcavity along the longitudinal optical axis. The microcavity consists of a flat mirror and a hemispherical mirror. Its shape can be characterised by three parameters,
TABLE I: Simulation results of complex reflectivities at central wavelength for Bragg mirrors with Ta$_2$O$_5$ being the layer of higher refractive index. The complex reflectivities at central wavelength is independent of the specific value of central wavelength.

| Media               | $N$ | $r$     | arg($\tilde{r}$)/rad |
|---------------------|-----|---------|-----------------------|
| SiO$_2$ + Ta$_2$O$_5$ | 8   | 0.995751 | 0                     |
| SiO$_2$ + Ta$_2$O$_5$ | 16  | 0.999991 | 0                     |
| Ta$_2$O$_5$ + SiO$_2$ | 8   | 0.995751 | $\pi$                 |
| Ta$_2$O$_5$ + SiO$_2$ | 16  | 0.999991 | $\pi$                 |

(1) the radius of curvature (RoC), $R$, of the spherical mirror

(2) length, $L$, separating the flat mirror and the top of the spherical mirror

(3) width $a$: the radius of the microcavity, which is also the distance from the central axis to the edge of the spherical mirror.

As we will see in Sec. III B, in order to have a stable cavity supporting a well defined mode, we must have $R > L$. For a given RoC $R$ and length $L$ satisfying this condition, the maximum possible width of the cavity is $a_{\text{max}} = \sqrt{R^2 - (R - L)^2} = \sqrt{2RL - L^2}$, when the edge of the spherical mirror is in contact with the flat mirror.

In our algorithm, if the input width $a_0$ is larger than the maximum possible width $\sqrt{2RL - L^2}$, we take the width of the microcavity to be the maximum possible width. Hence the width of the microcavity is

$$a = \min \left\{ a_0 , \sqrt{2RL - L^2} \right\} . \tag{16}$$

B. Gaussian Beam Mode

The electric field modes supported by the microcavity can be approximated by Gaussian beams. In principle, the electric field should be a vector field. But for our purpose to calculate the mode volume, a scalar description will be sufficient. We take the longitudinal optical axis as the $z$-axis of our coordinate, with the positive direction from the flat mirror to the spherical mirror, and leave its zero point (origin of the coordinate) unspecified for now. Notice that the system is rotationally symmetric about this axis.
FIG. 4. Cross-section through the microcavity along the longitudinal optical axis. Geometrical parameters $R$, $L$ and $a$ are indicated by arrows. The dashed line indicates the full circle of the upper spherical mirror with $R > L$ assumed.

If we define $\mathcal{E}(r)$ to be the spatial part of the electric field

$$E(r, t) = \mathcal{E}(r)e^{-i\omega t}$$  \hspace{1cm} (17)$$

then

$$\mathcal{E}(r) = \frac{A}{\sqrt{1 + z^2/z_0^2}} e^{ikz-\phi(z)} e^{ik(x^2+y^2)/2R(z)} e^{-(x^2+y^2)/(w(z)^2)}$$  \hspace{1cm} (18)$$

where $A$ is a constant coefficient, $\phi(z) = \arctan(z/z_0)$,

$$z_0 = \frac{\pi w_0^2}{\lambda}$$  \hspace{1cm} (19)$$

is the so-called Rayleigh range,

$$w(z) = w_0 \sqrt{1 + \frac{z^2}{z_0^2}}$$  \hspace{1cm} (20)$$

is the transverse width, or spot size, of the beam at $z$ and

$$R(z) = z + \frac{z_0}{z}$$  \hspace{1cm} (21)$$
is the radius of curvature of the wavefront [23, § 14.5]. It can be seen from Eq. (20) that $w_0$ is the minimum spot size of the beam. The electric field strength distribution of a typical Gaussian beam is shown in Fig. 5.

![Electric field strength distribution](image)

**FIG. 5.** Electric field strength distribution $\mathcal{E}(\mathbf{r})$ of a Gaussian beam with minimum waist $w_0 = 1.5 \lambda$. $\mathcal{E}(\mathbf{r})$ is in arbitrary unit (a.u.). The horizontal coordinate $r = \sqrt{x^2 + y^2}$. The Rayleigh range $z_0$ and minimum spot size $w_0$ are indicated by arrows. The two green curves indicate $r = \pm w(z)$. At $z = z_0$, $w(z) = \sqrt{2} w_0$. The plotting program is adapted from [24].

In Eq. (18), the term $\exp\{i[kz - \phi(z)]\}$ corresponds to a wave with wavelength $\lambda$ propagating in the $z$ direction. Wavefront of the beam at $z$ has radius of curvature $R(z)$ due to the term $\exp[i k (x^2 + y^2)/2R(z)]$. And the term $\exp[-(x^2 + y^2)/w^2(z)]$ tells us that the electric field strength decays exponentially in the lateral direction, by a factor of $e^{-1}$ when $r = w(z)$.

The constants $z_0$ and $w_0$ are related by Eq. (19). It follows that for a fixed wavelength $\lambda$, only $z_0$ or $w_0$ are adjustable parameters in the expression for the electric field in Eq. (18). These are related to the geometrical parameters of the cavity.

If a Gaussian beam is to be a mode of the microcavity, the radii of curvature of its wavefront at each mirror must equal that of the mirror. Otherwise the mirror would change the magnitude of the beam radius upon reflection [23, § 14.7] and a resonant standing wave could not be formed. We notice that the RoC of the beam at $z = 0$

$$R(0) = 0 + \frac{z_0^2}{0} \to \infty$$

and that the RoC of the flat mirror is also $\infty$. Therefore, $z = 0$ surface of the beam should
coincide with the flat mirror. I.e. origin of the coordinate is on the flat mirror. Then the center of the spherical mirror is at \( z = L \). And we should have

\[
R(L) = L + \frac{z_0^2}{L} = R.
\]

Hence

\[
z_0 = \sqrt{L(R - L)}
\]

and using Eq. (19),

\[
w_0 = \sqrt{\frac{\lambda}{\pi}} [L(R - L)]^{\frac{1}{2}}.
\]

To satisfy \( z_0 \), we must have

\[
R > L,
\]

which justifies the assumption we made for the geometry of the cavity in section III A. Using Eqs. (19) and (20), we can also write \( w(z) \) as

\[
w(z) = \sqrt{\frac{\lambda}{\pi}} \left( z_0 + \frac{z}{z_0} \right).
\]

The above expressions allow us to calculate the distribution of the electric field inside the cavity from its geometrical parameters.

### C. Resonant Frequency of the Cavity

The electromagnetic wave propagates forwards and backwards in the cavity upon reflection by the mirrors. To form a standing-wave, the field should be the same after it travels a round trip through the cavity. Therefore, the phase change of the field in a round trip should be integral multiple of 2\( \pi \). Now consider the phase of the wave along the \( z \)-axis

\[
\theta(z) = k z - \arctan(z/z_0).
\]

Hence the resonance condition can be written as

\[
2 (\theta(L) - \theta(0)) + \Delta \phi_1 + \Delta \phi_2 = 2q\pi \quad q \in \mathbb{N}_+.
\]

where \( \Delta \phi_1 \) and \( \Delta \phi_2 \) are the phase shifts induced upon reflection by the flat and spherical Bragg mirrors respectively. Using Eq. (22) and frequency \( \nu = kc/2\pi \), we can solve for resonant frequencies

\[
\nu_q = \frac{c}{2L} \left( q - \frac{\Delta \phi}{\pi} + \frac{1}{\pi} \arccos \sqrt{1 - L/R} \right).
\]
where $\Delta \phi \equiv (\Delta \phi_1 + \Delta \phi_2)/2$ is the mean phase shift. By choosing the first layers of the two Bragg mirrors to have either a high or low refractive index, we can set the values of $\Delta \phi_1$ and $\Delta \phi_2$ to be either 0 or $\pi$. As we will see, this choice is based on physical considerations, considering that a zero phase shift upon reflection will create an anti-node at the mirror surface whereas a phase shift of $\pi$ will create a node. Because the emitter is on the surface of the flat mirror, if we aim to increase the coupling between the emitter and the cavity mode, an anti-node should be at the flat mirror surface where the amplitude of the oscillating electric field is maximum. Thus layers of the flat mirror should start with the lower refractive index material imparting no phase shift ($\Delta \phi_1 = 0$) upon reflection.

Eq. (28) shows that for a microcavity of a given shape, only modes at certain frequencies can form resonances in the microcavity. For a given wavelength $\lambda$, the geometrical parameters of the microcavity must satisfy the condition

$$L = \frac{\lambda}{2} \left( q - \frac{\Delta \phi}{\pi} + \frac{1}{\pi} \arccos \sqrt{1 - \frac{L}{R}} \right).$$

This implicit condition is inconvenient to work with, since $L$ and $R$ can no longer be selected freely. To work around this limitation, we define two new variables, the effective mode number, $q_{\text{eff}}$, and the length-to-RoC ratio, $lr$, where

$$q_{\text{eff}} = q - \frac{\Delta \phi}{\pi}, \quad q \in \mathbb{N}_+$$

$$lr = \frac{L}{R} \in (0, 1)$$

assuming $R > L$ from Eq. (24). Then length $L$ and RoC $R$ can be expressed as

$$L = \frac{\lambda}{2} \left( q_{\text{eff}} + \frac{1}{\pi} \arccos \sqrt{1 - lr} \right)$$

$$R = \frac{\lambda}{2 lr} \left( q_{\text{eff}} + \frac{1}{\pi} \arccos \sqrt{1 - lr} \right)$$

The advantage of doing so is that the new variables $q_{\text{eff}}$ and $lr$ can now be chosen freely. Any combinations guarantee that the microcavity remains resonant with the Gaussian beam mode at the design wavelength.

**D. Quality Factor**

The quality factors of both the cavity and the emitter are defined as the central frequency divided by the full width half maximum (FWHM) frequency, which is equal to central wave-
length divided by the full width half maximum wavelength

\[ Q_i \equiv \frac{\nu_0}{\delta \nu_i} = \frac{\lambda_0}{\delta \lambda_i} \tag{34} \]

where \( i \) denotes the cavity or emitter and assumes that they are on resonance.

The spectrum of a given emitter depends only on its inherent optical properties so we assume a fixed quality factor, \( Q_{\text{em}} \), for the emitter.

The quality factor of the cavity depends on the design properties of its mirrors and their separations, and can be engineered to high values. To calculate the FWHM frequency of the cavity, we start from the expression of its transmission intensity \( I_T \). The dependence of \( I_T \) on the frequency detuning from mode \( q \), \( \Delta \nu_q = \nu - \nu_q \), is given by the Airy formula \[25, \S \ 1.2.1\]

\[ I_T (\Delta \nu_q) \propto \left[ 1 + \frac{4 \sqrt{R_1 R_2}}{(1 - \sqrt{R_1 R_2})^2} \sin^2 \left( \frac{\pi \Delta \nu_q}{\nu_{\text{FSR}}} \right) \right]^{-1} \tag{35} \]

where \( \nu_{\text{FSR}} \) is the free spectral range (FSR) of the cavity and is defined as the difference between the frequencies of two consecutive resonant modes

\[ \nu_{\text{FSR}} \equiv \nu_{q+1} - \nu_q = \frac{c}{2L} \tag{36} \]

and \( R_1, R_2 \) are amplitude reflectivities of the two mirrors. This formula is obtained through summing over amplitudes of all the transmitted electric field through the cavity which take the form of an infinite geometric series and then taking square modulus to get the intensity.

If the reflectivities of the mirrors are near-unity, the factor

\[ \frac{4 \sqrt{R_1 R_2}}{(1 - \sqrt{R_1 R_2})^2} \gg 1 \]

is very large. Therefore, when the transmission intensity drops to half its maximum value, the detuning frequency is

\[ \Delta \nu_q = \pm \frac{\nu_{\text{FSR}}}{2 \mathcal{F}} \]

where

\[ \mathcal{F} = \frac{\pi \sqrt{R_1 R_2}}{1 - \sqrt{R_1 R_2}} \tag{37} \]

is the finesse of the cavity. So the FWHM frequency of the cavity

\[ \delta \nu_{\text{cav}} = \frac{\nu_{\text{FSR}}}{\mathcal{F}} \tag{38} \]

and thus the quality factor of the cavity gives

\[ Q_{\text{cav}} = \frac{\nu_q}{\nu_{\text{FSR}}} \mathcal{F} = \mathcal{F} \left( q_{\text{eff}} + \frac{1}{\pi \sqrt{1 - l_T}} \right) \tag{39} \]
We note that the cavity decay rate $\kappa$ is related to its linewidth by $\kappa = 2\pi \nu_{cav}$. Using Eqs. (38,39), we have

$$\kappa = \frac{2\pi \nu_q}{Q_{cav}}$$

(40)

i.e. the decay rate of the cavity $\kappa$ is inversely proportional to the quality factor of the cavity.

Working in the weak coupling regime, we want the cavity decay rate to be large enough so as to be much higher than the coupling constant between the emitter and the cavity (as mentioned in Sec. I). As a result, quality factor of the cavity cannot be too high.

Since the effective quality factor of the cavity-emitter system $Q_{eff} = (Q^{-1}_{cav} + Q^{-1}_{em})^{-1}$, we will always have $Q_{eff} < \min\{Q_{em}, Q_{cav}\}$. If the cavity quality factor $Q_{cav}$ exceeds the quality factor of the emitter, $Q_{em}$, the effective quality factor will ultimately be limited by $Q_{em}$.

E. Mode Volume

The mode volume of the cavity-emitter system is defined as

$$V = \int \varepsilon_r(r)|E(r)|^2 d^3r$$

(41)

where $\varepsilon_r$ is the relative electric permittivity. On the right hand side, $|E(r)|$ is the magnitude of the electric field at position $r$ which is just $E(r,t)$ in our scalar description. Moreover, since standing wave is formed on resonance, electric field in the whole space oscillates in phase sinusoidally. The time-dependent factors in the numerator and denominator cancel out. In other words, mode volume of a standing wave mode is time-independent and we only need to focus on the spacial part of the electric field while calculating the mode volume.

In principle, the integral in Eq. (41) should be taken over all space. But since the transmittance of the Bragg mirrors are low, the magnitude of the electric field leaking out of the cavity is small compared with the field inside. In our algorithm, the integration region consists of the air gap between the mirrors and the layers of two Bragg mirrors.

Inside the air gap, the relative permittivity is uniformly equal to 1. Also, as seen in Sec. III C, when the resonance condition is met, a standing wave is formed in the air gap, so
the electric field is just the sum of travelling waves propagating forwards and backwards

\[ E_{\text{cav}} = \Re \left( \mathcal{E}(x, y, z)e^{-i\omega t} + \mathcal{E}(x, y, -z)e^{-i\omega t} \right) \]

\[ = \frac{2A}{\sqrt{1 + z^2/z_0^2}} \cos \left[ k z - \phi(z) + k \frac{x^2 + y^2}{2R(z)} \right] \times e^{-\left(x^2+y^2\right)/w^2(z)} \cos(\omega t) \]  

(42)

The field decays quickly as it penetrates into the Bragg mirrors, and in the air gap the maximum field strength \( \varepsilon_r |E|^2 \) occurs at the origin. If we take the coefficient \( A = 1/2 \), we simply have \( \max(\varepsilon_r |E|^2) = 1 \). Thus the mode volume in the air gap is

\[ V_{\text{air}} = \int_{\rho=0}^{a} \int_{z=0}^{L-R+\sqrt{R^2-\rho^2}} \mathcal{E}_{\text{cav}}^2 2\pi \rho \, d\rho \, dz \]  

(43)

where \( \rho = \sqrt{x^2 + y^2} \) and \( \mathcal{E}_{\text{cav}} \) is the spatial part of Eq. (42) with \( A = 1/2 \), i.e.

\[ \mathcal{E}_{\text{cav}} = \frac{1}{\sqrt{1 + z^2/z_0^2}} \cos \left[ k z - \phi(z) + k \frac{x^2 + y^2}{2R(z)} \right] \times e^{-\left(x^2+y^2\right)/w^2(z)}. \]  

(44)

To describe the mode volume due to the electric field penetrating into the layers of the Bragg mirror, we define several new variables. Regardless of whether the Bragg mirror starts with a high index layer \( (n_1 > n_2) \) or a low index layer \( (n_1 < n_2) \), let us assign the labels \( n_H \) and \( n_L \) for the higher and lower refractive indices respectively

\[ n_H = \max\{n_1, n_2\} \]  

(45)

\[ n_L = \min\{n_1, n_2\}. \]  

(46)

We also define

\[ \Delta n = n_H - n_L \]  

(47)

\[ \tilde{n} = \frac{2n_H n_L}{n_H + n_L} \]  

(48)

where the latter is the refractive index averaged by thicknesses of the Bragg mirror layers. The optical penetration depths of the electric field into the Bragg mirror are given by

\[ L_H = \frac{\lambda}{4\Delta n} \]  

(49)

\[ L_L = \frac{\tilde{n}^2 \lambda}{4\Delta n} + \frac{\Delta n \lambda}{2\pi^2} \]  

(50)
where $L_H$ ($L_L$) is the penetration depth into Bragg mirror starting with a high (low) index layer [26]. Since $\tilde{n} > 1$, we have $L_H < L_L$. Using this notation, the mode volume inside the two Bragg mirrors can be written as

$$V_{\text{pen}} = \frac{1}{4} \pi w_0^2 L_{\text{pen}}.$$  \hspace{1cm} (51)

where $L_{\text{pen}}$ is the total penetration depth into the two Bragg mirrors and can have values $2L_L$, $L_L + L_H$ or $2L_H$, depending on the starting layer of the mirrors. As we saw in Sec. III C, the flat mirror should start with a lower index layer, corresponding to an optical penetration depth $L_L$. To minimise the total mode volume (and hence to maximize the Purcell factor), we aim to use a spherical mirror with the lowest optical penetration depth, $L_H$. Hence, the spherical mirror should start with a high index layer, imparting a $\pi$ phase shift upon reflection.

To summarize, the total mode volume

$$V = V_{\text{air}} + V_{\text{pen}} = \int_{\text{gap}} \mathcal{E}_{\text{cav}}^2 \, d^3 r + \frac{\pi}{4} w_0^2 (L_L + L_H).$$ \hspace{1cm} (52)

The mean phase shift upon reflection $\Delta \phi = \pi/2$. Now, all the unknown elements on the RHS of Eq. (3) can be calculated and the Purcell factor $F_P$ can therefore be determined.

**F. Theoretical and Practical Limitations**

We can infer from Eq. (20) that the Gaussian beam widens as it propagates in the $z$ direction. If the Gaussian beam approximation is to hold, we must assume negligible leakage from the lateral sides of the cavity. This condition can be satisfied so long as the flat mirror is much wider than beam waist $w_0$, and the spherical mirror width, $a$, is several times larger than $w(z_a)$, where $w(z)$ is given by Eq. (20) and

$$z_a = -(R - L) + \sqrt{R^2 - a^2}$$

is the $z$ coordinate of the edge of the spherical mirror. Because the field strength of the Gaussian beam decreases exponentially in the lateral direction, $a$ only needs to be $3 \sim 5$ times $w(z_a)$, so that only a small fraction of incident of the beam is not reflected. In principle (albeit not in practice) this could be achieved by bringing the surfaces of the spherical mirror and the flat mirror into contact (i.e. by closing the cavity) so that all of the incident beam is reflected by the spherical mirror.
From a practical perspective, fabricating Bragg mirrors, especially the spherical mirror, imposes empirical limitations on the choice of geometrical parameters of the cavity. A hemispherical hole must first be milled into the surface of a substrate, which is then coated with alternate layers (SiO$_2$ and Ta$_2$O$_5$) to form a Bragg mirror. When the RoC of the spherical mirror $R$ is less than a few microns, the coating along the sharp rim of the mirror creates anisotropies in the coating, degrading the cavity’s quality factor and the curvature of the reflected wavefront, thus deviating from optimal resonance conditions. In practise, we choose the RoC to be within the range

$$5 \, \mu\text{m} \leq R \leq 15 \, \mu\text{m}.$$  \hspace{1cm} (53)

These considerations mean that we cannot set $lr$ very close to 1 (i.e. $R = L$). To see why, we consider the extreme scenario when $lr = 1$ (i.e. $R = L$). According to Eq. (22) if $R = L$ we have $z_0 = 0$. From Eq. (25) we find that $w(z) \to \infty$ as soon as $z > 0$, therefore we must close the cavity to avoid spillover. However, a closed cavity with $R = L$ is exactly half a sphere, so that the angle between the hemispherical surface and the surrounding flat surface is 90°, which is the most acute angle possible. These practical limitations restrict the range of RoC and the ratio $lr$.

IV. NUMERICAL RESULTS

Below we represent visually the distribution of the electric field in a hemispherical microcavity and of the Purcell factor. Numerical values of the parameters chosen in our computation are listed in Table II. Here, $\Delta \phi = \pi/2$ because the flat mirror imparts a phase shift $\Delta \phi_1 = 0$ upon reflection and the spherical mirror imparts $\Delta \phi_2 = \pi$ (see Sec. III C and III E). Furthermore, because $\Delta \phi = \pi/2$, the effective mode number, $q_{\text{eff}}$, can only take half-odd integer values (see Eq. (30) for the definition of $q_{\text{eff}}$).

TABLE II: Values of the parameters related to the microcavity and Bragg mirrors. $R_1$ is the intensity reflectivity of the flat mirror and $R_2$ is the intensity reflectivity of the spherical mirror.

| $\lambda$/nm | $\delta \lambda_{\text{em}}$/nm | $R_1$   | $R_2$   | $\Delta \phi$/rad |
|--------------|-----------------|--------|--------|-------------------|
| 537.0        | 2.5             | 0.999  | 0.970  | $\pi/2$           |
FIG. 6. (a) Intensity distribution of Gaussian beam mode ($\propto E_{\text{cav}}^2$) in the air gap of a cavity with mode number $q = 5$ and ratio $lr = 0.2$. (b) Refractive index and intensity distribution of the cavity mode along the central axis of the cavity with the same parameters. The intensity is in arbitrary unit (a.u.).

A. Electric Field Distribution

Figure 6a shows the distribution of electric field intensity, which is proportional to $E_{\text{cav}}^2$, inside a cavity with mode number $q = 5$ and ratio $lr = 0.2$. By design, the anti-node coincides with the flat mirror surface and the node coincides with the spherical mirror surface. We note that the shape of the wavefront on the spherical mirror conforms to its surface.

In Fig. 6b, the distribution of the electric field intensity and refractive indices along the z-axis are overlaid to illustrate the penetration of the field into Bragg mirror layers. We note that the penetration is deeper into the flat mirror (starting with a lower-index layer) compared to the spherical mirror (starting with a higher-index layer layer). This is qualitatively consistent with the theoretical analysis in Sec. III E where $L_H < L_L$. Furthermore, with this profile of electric field intensity, penetration depths can also be evaluated numerically. Result given by this alternative method agrees with those given by the theoretical formulae (Eqs. 49, 50) to high precision. (See Appendix A for detail.)
B. Purcell Factor

The distribution of the effective quality factor $Q_{\text{eff}}$ as a function of the effective mode number $q_{\text{eff}}$ and length-to-RoC ratio $lr$ is shown in Fig. 7a. Because the emitter has linewidth $\delta \lambda_{\text{em}} = 2.5 \text{ nm}$, its quality factor $Q_{\text{em}} = 214.8$. From Eq. (39), the cavity quality factor is roughly proportional to $q_{\text{eff}}$. But the maximum value of $Q_{\text{eff}}$ is limited by $Q_{\text{em}}$. As $q_{\text{eff}}$ increases, $Q_{\text{eff}}$ gradually saturates.

The distribution of mode volume $V$ is shown in Fig. 7b, where the maximum width of the cavity $a_0$ is fixed at 10 times the wavelength i.e. $a_0 = 5.37 \mu \text{m}$. $V$ increases with higher $q_{\text{eff}}$, however, unlike the quality factor $Q_{\text{eff}}$, the inverse dependence of $V$ on $lr$ is more significant. As $lr$ increases, $V$ decreases. This is because larger $lr$ makes the radius of curvature $R$ closer to length $L$, resulting in smaller beam width $w_0$. Electric field inside the cavity will decay faster laterally, which leads to smaller mode volume.

Fig. 7c shows the distribution of Purcell factor $F_P$ which is proportional to $Q_{\text{eff}}$ and to the reciprocal of $V$. As $q_{\text{eff}}$ gets larger, length $L$ increases and the increasing tendency of $Q_{\text{eff}}$ competes with that of $V$. But due to the reason that $Q_{\text{eff}}$ increases slower than $L$, whereas $V$ is roughly proportional to the actual volume of the cavity, which is about $L^3$, the latter is more dominant. Hence $F_P$ is large at small values of $q_{\text{eff}}$ and large values of $lr$ (where $V$ is small).

The Purcell factor $F_P$ is proportional to $Q_{\text{eff}}$ and to the reciprocal of $V$, the mode volume. $Q_{\text{eff}}$ varies more slowly with cavity length $L$ compared to the mode volume $V$, which is roughly proportional to the cavity’s length cubed, $L^3$ hence dominates. $F_P$ is large at small values of $q_{\text{eff}}$ and large values of $lr$ (when $V$ is small).

In Fig. 7c we identify the maximum Purcell factor achievable in the range of radius of curvature between $5 \mu \text{m} \leq R \leq 15 \mu \text{m}$. This is encompassed in the region between the two white dashed lines. The third row in Table III summarizes the values for the cavity’s geometrical parameters, the quality factor and mode volume, corresponding to the optimal Purcell factor.

C. Dependence of Purcell Factor on Wavelength

The quality factors ($Q_{\text{cav}}, Q_{\text{em}}, Q_{\text{eff}}$) and the Purcell factor, $F_P$, are all dimensionless, as is the ratio of mode volume to wavelength, $V/\lambda^3$. In our numerical computation, we used an
FIG. 7. The distribution of (a) the effective quality factor $Q_{\text{eff}}$, (b) the mode volume $V$ and (c) the Purcell factor, $F_P$, on the 2-D parametric space spanned by effective mode number $q_{\text{eff}}$ and the ratio $l/r$. In all figures, values are indicated by color and are higher in red regions. For (b) and (c), the maximum width of the cavity $a_0 = 5.37 \, \mu$m. In (a), $Q_{\text{eff}}$ increases together with $q_{\text{eff}}$ and is insensitive to $l/r$. In (b), $V$ increases with $q_{\text{eff}}$ and as $l/r$ decreases. In (c), $F_P$ is larger at smaller $q_{\text{eff}}$ and larger $l/r$. The two white dashed lines indicate the combinations of $q_{\text{eff}}$ and $l/r$ that correspond to a constant RoC for $\lambda = 537 \, \text{nm}$, with the upper line corresponding to $R = 5 \, \mu$m and the lower one to $R = 15 \, \mu$m. The region between them encompasses $5 \, \mu$m $\leq R \leq 15 \, \mu$m where the maximum $F_P$ is scanned for. (d) shows the same distribution in 3-D as (c).
TABLE III: Maximum Purcell factor and corresponding parameters.

| Parameters       | $\lambda$/nm | 537  | 1550 |
|------------------|--------------|------|------|
| $Q_{em}$         |              | 214.8| 214.8|
| $a_0/\mu$m       |              | 5.37 | 15.50|
| Location of Maxima | $q_{eff}$ | 1.5  | 1.5  |
|                  | $lr$         | 0.08563 | 0.2588 |
| Geometrical Parameters | $L/\mu$m | 0.4281 | 1.294 |
|                  | $R/\mu$m     | 5.000 | 5.000|
|                  | $a/\mu$m     | 2.024 | 3.357|
| Results          | $Q_{eff}$    | 128.3 | 130.7|
|                  | $V/\lambda^3$ | 1.482 | 0.8094|
|                  | $F_P$        | 6.58  | 12.3 |

arbitrary central wavelength of 537 nm, typical of certain semiconductor quantum dots. Let us now consider a different wavelength, say 1550 nm, which is a technologically important wavelength in the telecommunications band 1260 - 1620 nm. This will help us illustrate how the numerical results of the microcavity-emitter system might change with wavelength.

If the emitter quality factor, $Q_{em}$, and the ratio $a_0/\lambda$ remain unchanged, the dependence of $F_P$ (as well as $Q_{eff}$ and $V/\lambda^3$) on $q_{eff}$ and $lr$ will be independent of wavelength. Suppose that we fix the variables $q_{eff}$ and $lr$, and choose a different design wavelength that is $\alpha$ times the original value, $\lambda' = \alpha \lambda$. Since $Q_{cav}$ is independent of wavelength, a new emitter with a different wavelength will also leave $Q_{eff}$ unchanged (assuming the same $Q_{em}$). From Eqs. (31,32), we can see that $L$ and $R$ are proportional to wavelength, so they will be multiplied by the factor $\alpha$, and so are the parameters $z_0$ and $w_0$. In this way, if we take the new maximum width $a'_0 = \alpha a_0$, the cavity and the cavity mode will scale up isotropically by the factor $\alpha$. Thus we would expect the new mode volume to scale up by a factor of $\alpha^3$ and the quantity $V'/\lambda'^3 = V/\lambda^3$ to remain unchanged.

However, as the wavelength changes, the range of RoC (Eq. (53)) will shift to a different region on the $q_{eff} - lr$ plane corresponding to different values of the Purcell factor $F_P$. We assume the same the ratio $a_0/\lambda = 10$ as before, so that the dependence of $F_P$ on $q_{eff}$ and $lr$ remains unchanged.
The range of RoC \((5 \, \mu m \leq R \leq 15 \, \mu m)\) is encompassed in Fig. 7c in the region bounded by the two dashed orange lines. The maximum Purcell factor in this region at smaller \(lr\) and the corresponding parameters are listed in the fourth column in Table III. A second maximum at \(lr\) near 1 is omitted (see Sec. III F).

V. CONCLUSION

We presented a method for calculating the reflectivity of Bragg mirrors and built up a numerical model to compute the Purcell factor of a hemispherical microcavity with realistic parameters. The ordering of layers in the Bragg mirrors are chosen to minimise the mode volume and to maximise the Purcell factor. To ensure that the cavity is resonant with the emitter, two dimensionless variables - the effective mode number \(q_{\text{eff}}\) and the ratio \(lr\) - were introduced to replace the geometrical cavity parameters, length \(L\), and RoC \(R\). Finally, the maximum Purcell factor was calculated in the 2-D parametric space spanned by \(q_{\text{eff}}\) and \(lr\), and the corresponding optimal cavity parameters were identified. Our numerical model employed quantities that are wavelength-independent, including the reflectivity of Bragg mirror and the Purcell factor. Parameters such as the central design wavelength and the quality factor of the emitter can readily be incorporated into the model, making it versatile and relevant for systems with different parameters.

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APPENDIX

A. Numerical Evaluation of Penetration Depth

Recall that the spatial part of the electric field distribution in the air gap of the cavity is

$$E_{\text{cav}} = \frac{1}{\sqrt{1 + \frac{z^2}{z_0^2}}} \cos \left[ kz - \phi(z) + k \frac{x^2 + y^2}{2R(z)} \right]$$

$$\times e^{-\left(\frac{x^2+y^2}{w^2}\right)}/w(z). \quad (44\text{ revisited})$$

We assume that when the electric field penetrates into the dielectric stacks, its transverse distribution

$$E_{\perp}(x, y, z) = \frac{1}{\sqrt{1 + \frac{z^2}{z_0^2}}} e^{-\left(\frac{x^2+y^2}{w^2}\right)}/w(z)$$

does not change, while its longitudinal distribution of intensity $E_{\parallel}^2(z)$ is that shown in Fig. 6b.

We also neglect the curvature of the spherical mirror. This is justified since the intensity is negligible after a few (4 to 5) layer pairs. Therefore, the mode volume in one DBR is

$$V_{\text{pen}} = \int \int \int \epsilon E^2 \, dV$$

$$= \int \int E_{\perp}^2(x, y, z) \, dx \, dy \int n^2 E_{\parallel}^2(z) \, dz$$

$$\pi w_0^2/2$$

$$= \frac{1}{4} \pi w_0^2 \times 2 \int n^2 E_{\parallel}^2(z) \, dz.$$

Compared with Eq. (51), we can read the penetration depth as

$$L_{\text{pen}} = 2 \int E_{\parallel}^2(z) \, dz. \quad (54)$$

Values of penetration depths into the flat and spherical Bragg mirrors obtained from analytical expressions Eqs. (49,50) and numerically evaluating Eq. (54) are shown in Table IV. The discrepancies are less than 1%.
TABLE IV: Comparison between penetration depths from calculating Eqs. (49, 50), $L_{\text{pen}}^{(\text{theo})}$, and computing Eq. (54) numerically, $L_{\text{pen}}^{(\text{num})}$, for both the flat and spherical Bragg mirrors.

| Mirror     | Media           | $N$ | $L_{\text{pen}}^{(\text{theo})}/\lambda$ | $L_{\text{pen}}^{(\text{num})}/\lambda$ |
|------------|-----------------|-----|----------------------------------------|----------------------------------------|
| Flat       | SiO$_2$+Ta$_2$O$_5$ | 16  | 1.137                                  | 1.144                                  |
| Spherical  | Ta$_2$O$_5$+SiO$_2$ | 8   | 0.3651                                 | 0.3628                                 |