Super-collimation with high frequency sensitivity in 2D photonic crystals induced by saddle-type van Hove singularities

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Abstract: Using detailed numerical simulations, and theoretical modeling, we predict a new super-collimation operation regime which is very sensitive on frequency. This operation regime is predicted to exist in 2D photonic crystals of dielectric rods in low index media. We explain the physical origin of this operation regime, as well as discuss how it could be of interest for implementation of low-power non-linear devices, novel sensors, as well as low-threshold lasers.

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1. Introduction

During the last two decades, photonic crystals (PhCs) [1,2] have been used to implement numerous micro optical devices with outstanding performance, in many cases due to their rich and engineerable dispersion relations. Among them, super-collimation (SC) [3–16], which is associated with a zero-curvature segment of the equi-frequency-contour (EFC), resulting in non-diffracting beams, has been intensively studied. SC originates from the fact that group velocities of Bloch modes are perpendicular to the EFC, so that the modes within the flat EFC segment all propagate in the same direction, as thus the diffraction is eliminated. As a boundary-less waveguiding mechanism, SC proved to be promising in implementing micro optical devices: beam splitters [7–9], interferometers [10], filters [11], polarization splitters [12,13], etc. The robustness of SC has been verified via centimetre scale experiments in a silicon platform [14–16]. SC has also been found in layered PhCs, as well as in metamaterial systems [17–20].

Generally, SC is strictly valid only at a specific frequency $\omega_{sc}$, where the EFC curvature is identically zero. Around $\omega_{sc}$, there is a frequency range where the EFC curvature is close to zero, so that SC is a good approximation also within this frequency range. We define the frequency sensitivity of SC (FSSC) as the rate of change of EFC curvature with respect to $\omega$ around $\omega_{sc}$. For some applications, large bandwidth approximate-SC has drawn a substantial interest since it allows transmission of polychromatic light and supports more signal channels [21–23]. However, for certain other applications, extremely narrow approximate-SC frequency range, with low group velocity $\upsilon_g$ is more useful. Examples include devices which explore interplay between SC and nonlinearity [24–27], or those that explore laser design with SC [28–30]. In other words, high FSSC is desired: in that case, the curvature of EFCs strongly deviates from zero when the working frequency $\omega$ is even only a little bit different from $\omega_{sc}$.

To appreciate why high FSSC is of interest in the interplay between SC and nonlinearity consider the following. First, suppose that the PhC comprises a nonlinear material, and that the incident beam frequency is near $\omega_{sc}$ of the PhC. Second, the large intensity of the incident beam (or external pumping light) can cause a nonlinear index change, so that $\omega_{sc}$ is shifted. Thereby, the curvature values (even their sign) of all the nearby EFSs (which determines the beam diffraction behavior), could be substantially modulated. Hence, new phenomena and devices could be implemented, such as tunable or self-locked beam-width [25], spatial-temporal soliton [27] and ultra fast optical switches [28]. Since the nonlinear index change is very small, one generally needs the EFC curvature around $\omega_{sc}$ to be very sensitive to frequency in order to observe considerable beam-modulation effects. In a similar way, when one aims to explore low-loss SC beam to design new free-path lasers [28], FSSC will enhance the cavity quality factor and facilitate the single-mode behavior. Therefore, high FSSC could be quite useful for light behavior modulation and lasing cavity design near $\omega_{sc}$. Moreover, with high FSSC, other devices, such as extremely sensitive micro-scale on-chip spectrometers could be implemented. However, to the best of our knowledge, a detailed study of how to improve FSSC is still lacking.

In this article, we show that SC of an extremely high frequency sensitivity could be achieved in 2D rectangular lattice PhCs which consist of dielectric rods in air. This phenomena is mainly caused by saddle-type van Hove singularities [31]. First, we show theoretically that the frequency sensitivity of the EFS curvature close to $\omega_{sc}$ is strongly enhanced as the group velocity becomes small. Second, we demonstrate that saddle-type van Hove singularities, i.e., points with zero group velocity, can be tuned arbitrarily close to $\omega_{sc}$ by reducing the symmetry of the lattice type and changing the aspect ratio of the lattice constants, so that an extremely-high-sensitivity SC is obtained. In addition, by analysing the spatial distribution of the Poynting vectors of the Bloch modes associated with such high FSSC, we can explain why such extremely sensitive SC can exist widely in the multi-parameter space of PhC design, and why this phenomenon is very robust. Finally, we propose a few different possible applications of high...
2. Models and theory

We start by analyzing the EFCs close to $\omega_c$ in Fig. 1 for the second $TE$ band of two $2D$ square-lattice PhCs, whose vertical dimension is assumed to be infinite; from this, we can obtain some clues about the properties of FSSC. Figure 1(a) corresponds to the holes of air in a dielectric background type (hole-type) PhC and Fig. 1(b) corresponds to the rods of dielectric in air background type (rod-type) PhC. The radius of both air holes and dielectric rods are the same in these two examples: $r = 0.30a$, where $a$ is the lattice constant. The dielectric materials in both PhCs are also the same: $n_d = 3.4$. From Fig. 1, we can roughly estimate that the FSSC of rod-type PhC is much higher than that of hole-type, since the frequency difference between the neighbouring EFCs around $\omega_c$ in Fig. 1(b) is 0.002$(2\pi c/a)$, while in Fig. 1(a) it is 0.02$(2\pi c/a)$. Notice the presence of saddle-type van Hove singularities, not as $S_1$ (red diamonds) in Fig. 1(b); they are absent in Fig. 1(a). In what follows, we will derive a quantitative expression of FSSC and reveal that such singularities are essential for implementing high FSSC.

From now on, we will denote the central point of SC EFC segment at $\Gamma X$ axis in Fig. 1 as the “SC point”, and all the physical values will be defined around the SC point. Within the paraxial approximation, the physical quantity that measures the strength of FSSC is defined as:

$$\gamma = \frac{dk_0}{d\omega}|_{\omega=\omega_c}$$  \hspace{1cm} (1)

where $k_0 = (1/2)(\partial^2 k_x/\partial k_y^2)|_{k_y=0}$ is the EFC curvature along the $\Gamma X$ axis [32], which can also be expressed as [33]:

$$k_0 = \frac{\omega_{yy}}{\omega_x}|_{k_y=0}$$  \hspace{1cm} (2)

the subscripts after commas denote partial derivatives with respect to $k$ components: e.g. $\omega_x = \frac{d\omega}{dk_x}$ and $\omega_{yy} = \frac{\partial^2 \omega}{\partial k_y^2}$. Substituting Eq. (2) into Eq. (1), we obtain:

$$\gamma = \frac{dk_0}{dk_x} \frac{\partial \omega}{\partial k_x}|_{k_y=0,\omega=\omega_c} = \frac{\omega_{yy}}{\omega_x^2}|_{k_y=0,\omega=\omega_c}$$  \hspace{1cm} (3)

Because $k_0 = 0$ for the SC point (with $\omega = \omega_c$ and $k_y = 0$), it follows that:

$$\gamma = \frac{\omega_{yy}}{\omega_x^2}|_{\omega=\omega_c, k_y=0} = \frac{\omega_{yy}}{v_g^2}|_{\omega=\omega_c, k_y=0}$$  \hspace{1cm} (4)

Since $\omega_{yy}$ is finite and slowly-varying in our PhCs, Eq. (4) is indicative that FSSC is hugely enhanced in PhCs in which group velocity is small at the SC point. Using Eq. (4) and applying finite difference approximation with step $\Delta k_x = 0.002(2\pi c/a)$ and $\Delta k_y = 0.01(2\pi c/a)$, we compute the values of $\gamma$ for the hole-type and rod-type PhCs from Fig. 1, which are 75.1$(a^2/4\pi^2 c)$ and 1047.4$(a^2/4\pi^2 c)$, respectively, thus confirming quantitatively that FSSC is substantially higher in rod-type PhCs. Actually, difference of FSSC between hole-type and rod-type PhCs is also mentioned for the first TM band previously [34], but the difference is much smaller compared to ours since both of them are lacking of saddle-type van Hove singularities.

From further numerical investigations of various kinds of PhCs, we noticed that when there are saddle-type van Hove singularities near the SC frequency, the FSSC is greatly enhanced. This can be understood from Eq. (4) because the saddle-type van Hove singularity is characterized by zero group velocity. We can explore this understanding to propose a strategy for further
improvement of FSSC. In particular, one way to enhance $\gamma$ is to bring the saddle-type van Hove singularities $S_1$ closer to the SC point. However, due to the requirement of symmetry, $S_1$ singularities of a square lattice are constrained to be on the $\Gamma M$ axis [31]. Therefore, we need to reduce the symmetry of the lattice. A simple way to do this is to change the square lattice into a rectangular lattice, whose lattice constants are $a$ and $b$, in $x$ and $y$ directions, respectively. We find that the position of $S_1$ singularities strongly depends on the ratio $\beta = b/a$. More significantly, with a proper value of $\beta$, $S_1$ singularities can even be tuned arbitrarily close to the SC point, so that an extremely high FSSC can be achieved.

We start with the rod-type PhC from Fig. 1(b), and change $b$ to vary $\beta$ from 1.0 to 2.0: A few resulting EFCs around $\omega_{sc}$, as well as the corresponding movement of the singularities are shown in Fig. 2. As can be seen in Fig. 2(a), with $\beta = 1.2$, the $S_1$ singularities start to deviate away from the $\Gamma M$ axis and move towards the $\Gamma X_1$ axis. As we see in Fig. 2(b), a local maximum point $S_2$ (originating from the $\Gamma$ point of the square lattice), which is also characterized by zero group velocity, moves towards the SC point along the $\Gamma X_1$ axis as $\beta$ increases. Before they merge, these three zero-group-velocity points form the basic feature of the EFCs around the SC segment, which is indicated by the dashed two-arrow lines in Fig 2(a) and Fig. 2(b). Note that the angle range of the SC is reduced when the three singularities approach the SC point. In Fig. 2(c) with $\beta = 1.5$, all three singularity points are very close to the SC point and the angle range of SC is very small. We can expect that there is a critical case, when $\beta$ equals to a specific critical value $\beta_c$ close to 1.5, such that the singularity points are arbitrarily close to the SC point. The most interesting phenomena happen when $\beta$ is larger than $\beta_c$. For example, observe the case when $\beta = 1.6$ as in Fig 2(d), where the three singularity points have merged into one saddle-type van Hove point on the $\Gamma X_1$ axis, resulting in the appearance of SC EFC which extends through the entire BZ, meaning that the beam can be collimated at all angles [35]. FSSC in Fig. 2(d) is quite high, as the EFC curvature changes considerably even with frequency change smaller than 0.1%. For even larger $\beta$, as in Fig. 2(e) and Fig. 2(f), we can see that FSSC is substantially reduced compared with Fig. 2(d), but is still considerably high compared with typical PhCs.

Figure 3 displays $\gamma$ and $\nu_g$ at the SC point versus $\beta$. As we have theoretically predicted in Eq.

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Fig. 1. Diagrams of EFCs within the half Brillouin zone in the second TE band of two 2D square lattice PhCs. (a) corresponds to air holes PhC in dielectric background, while (b) corresponds to dielectric rods PhC in air background. In both Figs., the flat segment of the EFC representing SC is highlighted by a dashed double arrow, and the central point of such a segment is called the SC point. The red diamond point labelled as $S_1$ in (b) is a saddle-type van Hove singularity.
(4), it is clear that, as group velocity approaches zero, $\gamma$ is dramatically enhanced, and becomes divergent at the critical point with $\beta_c = 1.51$. If the operating wavelength is assumed to be 1550 nm, the fact that the experimental accuracy of modern semiconductor techniques is about $\pm 5$ nm implies that the accuracy of experimentally achieving a targeted $\beta$ is better than 0.01. Hence, from Fig. 3, we can see that the value of $\gamma$ could be as high as $10^7 (a^2/4\pi^2 c)$, which is 5 orders of magnitude larger than the common case (e.g. Fig. 1(a)). Even with $\beta = 1.6$ as in Fig. 2(d), $\gamma = 4 \times 10^4 (a^2/4\pi^2 c)$ which is about 600 times higher than Fig. 1(a).

We need to emphasize that the extremely high FSSC is not an anomalous phenomenon which only exists in a very small multi-parameter space. Quite on the contrary, we found that it exists in a very wide range of structures: *i.e.* rod index $3.4 > n_d > 3$, radius $0.45a > r > 0.2a$ and lattice aspect ratio $2.0 > \beta > 1.3$. The fact that this phenomenon exists in such a large multi-parameter space greatly facilitates the possibility of optimizing designs for different applications.

3. Origin of high FSSC and the flexible dual-vortex form of Bloch waves

Highly sensitive phenomena in physics are usually not robust, and typically do not exist over a large multi-parameter space; it is natural to wonder what is the physical origin of high FSSC
that we described in this manuscript. To achieve extremely sensitive and broad-angle SC, there are two conditions that must be satisfied simultaneously, (i) the group velocity in y-direction has to be close to zero $v_{gy} \approx 0$ along the entire SC EFC even when $k_y$ is far from zero, (ii) the group velocity at the SC point in x-direction has to be very low: $v_{gx} \ll c/n$ according to Eq. (4).

Group velocity behavior can be understood by analyzing the local Poynting vector $S(r)$ in a unit cell of PhC, since $v_{g} = \int d^2r S(r)/\int d^2r U(r)$ [36], where $U(r)$ is the energy density, and the integration is over the unit cell. In Fig. 4, we show the spatial distributions $S(r)$ of two Bloch modes: with $k_y = 0$ (the SC point), and $k_y = 0.1 \cdot 2\pi/b$, on the SC EFC of the case in Fig. 2(d), where $\beta = 1.6$. For the mode with $k_y = 0$ in Fig. 4(a), one can see formation of dual-vortex in $S$: we will show that this is the origin of high FSSC. The requirement $v_{gy} = 0$ is automatically satisfied because of the up-down symmetry. The reason for the low $v_{gx}$ is also clear, since the Poynting vector in the central part of the cell (with $y \sim 0$) is pointing towards the left direction, while in the upper and the lower parts it is pointing towards right: this way they can almost cancel each other. Such cancellation also reveals why it that we can obtain an extremely high FSSC by tuning only $\beta$. When we increase the lattice constant $b$ in the $y$-direction, the existence of dual-vortices persists, but the relative area of the upper and the lower parts increases; in other words, the right-going energy current becomes stronger and stronger. When the right-going current in the upper and the lower parts cancel the left-going current in the central part, the group velocity decreases to zero, and the extremely high FSSC appears.

In Fig. 4(b) with $k_y = 0.1 \cdot 2\pi/b$, the dual-vortex form gets modified by rotation through an angle since the up-down symmetry is now broken. Such rotation of dual-vortex does not change much the total energy current in the $y$-direction, so $v_{gy}$ remains close to zero. Moreover, such a rotation will increase the total current in the x-direction slowly, so that $v_{gx}$ increases with larger $k_y$, which can also be seen in Fig. 2(d). We have also investigated modes with even larger $k_y$: dual-vortex form rotates by an even larger angle. Actually, the dual-vortex form is very typical for Bloch modes in this band, and this explains the large multi-parameter space in which high FSSC exists. The flexibility of the dual-vortex form also provides intuition why high FSSC is so robust. Therefore, we can understand the origin of high FSSC through the existence of the dual-vortex form of the relevant Bloch modes.
Fig. 4. Spatial flux distributions within one unit cell, for modes of $\omega_c$ in 2D rectangular rod-typed PhCs with $r = 0.30a$ and $\beta = 1.6$. (a) corresponds to the SC point with $k_\parallel = 0$, while (b) corresponds to $k_\parallel = 0.1(2\pi/b)$. In each Fig., the dashed circle represents the boundary of the dielectric rod.

4. Summary and discussion

In summary, we have described SC with frequency sensitivity enhanced by several orders of magnitude, in 2D rectangular lattice PhCs consisting of dielectric rods. This phenomenon can be mainly attributed to saddle points that are present close to the SC point, which reduce the group velocity at the SC point. The relation between the group velocity at the SC point and the frequency sensitivity of SC is revealed by an analytical expression (Eq. (4)). The underlying physical mechanism that explains why the SC point and the saddle point could be brought arbitrarily close is well explained by inspecting the dual-vortex spatial flux distribution.

Range of possible applications of SC with very low group velocity and extremely high frequency sensitivity is very wide. As we mentioned before, new nonlinear devices, such as ultrafast switches, or self-locked beam modulators could be designed. In these devices, the diffraction behavior of micro-beams could be modified considerably with even a small nonlinear index change. Novel low threshold lasers could also be enabled since a low group velocity SC beam is an ideal base for micro-beam lasers. Sensors with extremely high sensitivity of small index change could also be implemented, as well as very compact spectrometers.

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