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High-efficiency degenerate four-wave mixing in triply resonant nanobeam cavities

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Using a combination of temporal coupled-mode theory and nonlinear finite-difference time-domain (FDTD) simulations, we study the nonlinear dynamics of all-resonant four-wave mixing processes and demonstrate the possibility of achieving high-efficiency limit cycles and steady states that lead to ∼100% depletion of the incident light at low input (critical) powers. Our analysis extends previous predictions to capture important effects associated with losses, self- and cross-phase modulation, and imperfect frequency matching (detuning) of the cavity frequencies. We find that maximum steady-state conversion is hypersensitive to frequency mismatch, resulting in high-efficiency limit cycles that arise from the presence of a homoclinic bifurcation in the solution phase space, but that a judicious choice of incident frequencies and input powers, in conjunction with self-phase and cross-phase modulation, can restore high-efficiency steady-state conversion even for large frequency mismatch. Assuming operation in the telecom range, we predict close to perfect quantum efficiencies at reasonably low ∼50 mW input powers in silicon micrometer-scale PhC nanobeam cavities.

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I. INTRODUCTION

Optical nonlinearities play an important role in numerous photonic applications, including frequency conversion and modulation [1–7], light amplification and lasing [1,8–10], beam focusing [1,11], phase conjugation [1,12], signal processing [13,14], and optical isolation [15,16]. Recent developments in nanofabrication are enabling fabrication of nanophotonic structures, e.g., waveguides and cavities that confine light over long times and small volumes [17–21], minimizing the power requirements of nonlinear devices [22,23] and paving the way for novel on-chip applications based on all-optical nonlinear effects [18,24–33]. In addition to greatly enhancing light-matter interactions, the use of cavities can also lead to qualitatively rich dynamical phenomena, including multistability and limit cycles [34–40]. In this paper, we explore realistic microcavity designs that enable highly efficient degenerate four-wave mixing (DFWM) beyond the undepleted pump regime. In particular, we extend the results of our previous work [41], which focused on the theoretical description of DFWM in triply resonant systems via the temporal coupled-mode theory (TCMT) framework, to account for various realistic and important effects, including linear losses, self-phase and cross-phase modulation, and frequency mismatch. Specifically, we consider the nonlinear process depicted in Fig. 1, in which incident light at two nearby frequencies, a pump ωp and signal ωm = ω0 − Δω photon, is up-converted into output light at another nearby frequency, an idler ωi = ω0 + Δω photon, inside a triply resonant photonic crystal nanobeam cavity (depicted schematically in Fig. 2). We demonstrate that 100% conversion efficiency (complete depletion of the pump power) can be achieved at a critical power and that detrimental effects associated with self-phase and cross-phase modulation can be overcome by appropriate tuning of the cavity resonances. Surprisingly, we find that critical solutions associated with maximal frequency conversion are ultraselective to frequency mismatch (deviations from perfect frequency matching resulting from fabrication imperfections), but that there exist other robust, dynamical states (e.g., “depleted” states and limit cycles) that, when properly excited, can result in high conversion efficiencies at reasonable pump powers. We demonstrate realistic designs based on PhC nanobeam cavities that yield 100% conversion efficiencies at ∼50 mW pump powers and over broad bandwidths (modal lifetimes Q ∼ 1000 s). Although our cavity designs and power requirements are obtained using the TCMT framework, we validate these predictions by checking them against rigorous, nonlinear finite-difference time-domain (FDTD) simulations.

Although chip-scale nonlinear frequency conversion has been a topic of interest for decades [33], most theoretical and experimental works have been primarily focused on large-etalon and singly resonant systems exhibiting either large footprints and small bandwidths [25,26,42,43], or low conversion efficiencies (the undepleted pump regime) [22,44–46]. These include studies of χ(2) processes such as second harmonic generation [26,47–49], sum and difference frequency generation [50], and optical parametric amplification [27,28,51], as well as χ(3) processes such as third harmonic generation [47,52], four-wave mixing [53–55], and optical parametric oscillators [22,56–58]. Studies that go beyond the undepleted regime and/or employ resonant cavities reveal complex nonlinear dynamics in addition to high-efficiency conversion [23,37–39,41,59,60], but have primarily focused on ring-resonator geometries due to their simplicity and high degree of tunability [60]. Significant efforts are underway to explore similar functionality in wavelength-scale photonic components (e.g., photonic crystal cavities) [49,50], although high-efficiency conversion has yet to be experimentally demonstrated. Photonic crystal nanobeam cavities not only offer a high degree of tunability, but also mitigate

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the well-known volume and bandwidth tradeoffs associated with ring resonators [61], yielding minimal device footprint and on-chip integrability [62,63], in addition to high-quality factors [21,64–67].

In what follows, we investigate the conditions and design criteria needed to achieve high-efficiency DFWM in realistic nanobeam cavities. Our paper is divided into two primary sections. In Sec. II, we revisit the TCMT framework introduced in Ref. [41], and extend it to include additional effects arising from cavity losses (Sec. II A), self-phase and cross-phase modulation (Sec. II B), and frequency mismatch (Sec. II C).

In Sec. III, we consider specific designs, starting with a simple two-dimensional (2D) design (Sec. III A) and concluding with a more realistic three-dimensional (3D) design suitable for experimental realization (Sec. III B). The predictions of our TCMT are checked and validated in the 2D case against exact nonlinear FDTD simulations.

II. ANALYSIS VIA TEMPORAL COUPLED-MODE THEORY

To obtain accurate predictions for realistic designs, we extend the TCMT predictions found in Ref. [41] to include important effects associated with the presence of losses, self-phase and cross-phase modulation, and imperfect frequency matching. We consider the DFWM process depicted in Fig. 1, in which incident light from some input or output channel (e.g., a waveguide) at frequencies $\omega_0$ and $\omega_p$ is converted to output light at a different frequency $\omega_m = 2\omega_0 - \omega_p$ inside a triply resonant cavity. The fundamental assumption of TCMT (accurate for weak nonlinearities) is that any such system, regardless of geometry, can be accurately described by a few sets of geometry-specific parameters [41]. These include the frequencies $\omega_{ka}$ and corresponding lifetimes $\tau_k$ (or quality factors $Q_k = \omega_k/\tau_k$) of the cavity modes, as well as nonlinear coupling coefficients $\alpha_{kk}$ and $\beta_k$, determined by overlap integrals between the cavity modes (and often derived from perturbation theory [23]). Note that, in general, the total decay rate (1/$\tau_k$) of the modes consist of decay into the input or output channel (1/$\tau_k$), as well as external (e.g., absorption or radiation) losses with decay rate 1/$\tau_k$, so that 1/$\tau_k = 1/\tau_{ek} + 1/\tau_{sk}$. Letting $\tau_{ek}$ denote the time-dependent complex amplitude of the $k$th cavity mode (normalized so that $|\tau_{ek}|^2$ is the electromagnetic energy stored in this mode), and letting $\tau_{sk}$ denote the time-dependent amplitude of the incident (+) and outgoing (−) light (normalized so that $|\tau_{sk}|^2$ is the power at the incident or output frequency $\omega_k$), it follows that the field amplitudes are determined by the following set of coupled ordinary differential equations [23]:

$$\frac{da_0}{dt} = i\omega_c a_0 (1 - |\alpha_0|^2 - |\alpha_m|^2 - |\alpha_p|^2) a_0$$

$$- \frac{a_0}{\tau_0} - i\omega_c \beta_0 a_0^* a_p + \frac{2}{\tau_{s0}} s_{0+},$$

$$\frac{da_m}{dt} = i\omega_c a_m (1 - |\alpha_m|^2 - |\alpha_p|^2) a_m$$

$$- \frac{a_m}{\tau_m} - i\omega_c \beta_m a_m^2 a_p + \frac{2}{\tau_{sm}} s_{m+},$$

$$\frac{da_p}{dt} = i\omega_c a_p (1 - |\alpha_p|^2 - |\alpha_m|^2 - |\alpha_p|^2) a_p$$

$$- \frac{a_p}{\tau_p} - i\omega_c \beta_p a_p^2 a_m^*,$$

$$s_{0-} = \sqrt{\frac{2}{\tau_{s0}}} a_0 - s_{0+},$$

$$s_{m-} = \sqrt{\frac{2}{\tau_{sm}}} a_m - s_{m+},$$

$$s_{p-} = \sqrt{\frac{2}{\tau_{sp}}} a_p.$$
where the nonlinear coupling coefficients \[41\]
\[
\alpha_{kk} = \frac{1}{8} \int d^3 \chi \alpha^{(3)} [2|E_k|^2 + |E_k \cdot E_k|^2] \left( \int d^3 \chi |E_k|^2 \right)^2 ,
\]
\[
\alpha_{kk'} = \frac{1}{4} \int d^3 \chi \alpha^{(3)} [|E_k|^2 + |E_k \cdot E_k|^2 + |E_k|^2 |E_k'|^2] \left( \int d^3 \chi |E_k|^2 \right)^2 ,
\]
\[
\alpha_{kk''} = \alpha_{kk'},
\]
\[
\beta_0 = \frac{1}{4} \int d^3 \chi \alpha^{(3)} [(E_m^0 \cdot E_p^0)(E_m \cdot E_p) + 2(E_m^0 \cdot E_m)(E_m^0 \cdot E_p)] \left( \int d^3 \chi |E_m|^2 \right)^2 \left( \int d^3 \chi |E_p|^2 \right)^2 ,
\]
\[
\beta_m = \beta_p = \beta_0 / 2 ,
\]

express the strength of the nonlinearity for a given mode, with the \[\alpha\] terms describing self-phase modulation (SPM) and cross-phase modulation (XPM) effects and the \[\beta\] terms characterizing the energy transfer between the modes. (Technically speaking, this qualitative distinction between \(\alpha\) and \(\beta\) is only true in the limit of small losses \[23\]).

A. Losses

Equations (1) and (4) can be solved to study the steady-state conversion efficiency of the system \([\eta = \text{losses} / (\text{losses} + \text{gain})]\) in response to incident light at the resonant cavity frequencies \((\omega_m = \omega_p)\), as was done in Ref. \[41\] in the ideal case of perfect frequency matching \((\omega_p = 2\omega_m - \omega_m)\), no losses \((\tau_\epsilon = \tau_{sk})\), and no SPM or CPM \((\alpha = 0)\). In this ideal case, one can obtain analytical expressions for the maximum efficiency \(\eta^{\text{max}}\) and critical powers \(P_0^{\text{crit}} = |s_\eta^{\text{crit}}|^2\) and \(P_m^{\text{crit}} = |s_m^{\text{crit}}|^2\), at which 100% depletion of the total input power is attained \[41\]. Performing a similar calculation, but this time including the possibility of losses, we find
\[
P_0^{\text{crit}} = \frac{4}{\tau_\epsilon |\beta_0| \sqrt{\tau_p / \tau_\epsilon \tau_\epsilon \tau_\epsilon \tau_{sk}}},
\]
\[
\eta^{\text{max}} = \frac{\tau_p}{\tau_{sk}} \left( 2 - \frac{\tau_\epsilon}{\tau_d} \right) \frac{\omega_p}{2\omega_0} .
\]

With respect to the lossless case, the presence of losses merely decreases the maximum achievable efficiency by a factor of \(\tau_p / \tau_{sk}(2 - \tau_\epsilon / \tau_d)\) while increasing the critical power \(P_0^{\text{crit}}\) by a factor of \(\sqrt{\tau_p / \tau_\epsilon \tau_\epsilon \tau_\epsilon \tau_{sk}}.\) As in the case of no losses, 100% depletion is only possible in the limit as \(P_m^{\text{crit}} \rightarrow 0\), from which it follows that the maximum efficiency is independent of \(P_m^{\text{crit}}.\) As noted in Ref. \[41\], the existence of a limiting efficiency \[11\] can also be predicted from the Manley-Rowe relations governing energy transfer in nonlinear systems \[68\] as can the limiting condition \(P_m^{\text{crit}} \rightarrow 0\). While theoretically this suggests that one should always employ as small a \(P_m^{\text{crit}}\) as possible, as we show below, practical considerations make it desirable to work at a small but finite \(P_m^{\text{crit}}.\)

B. Self-phase and cross-phase modulation

Unlike losses, the presence of SPM and XPM dramatically alters the frequency-conversion process. Specifically, a finite \(\alpha\) leads to a power-dependent shift in the effective cavity frequencies \(\omega_k^{\text{crit}} = \omega_k(1 - \sum \alpha_k |A_j|^2)\) that spoils both the frequency-matching condition as well as the coupling of the incident light to the corresponding cavity modes. One approach to overcome this difficulty is to choose or design the linear cavity frequencies to have frequency \(\omega_k\) slightly detuned from the incident frequencies \(\omega_0\), such that at the critical powers the effective cavity frequencies align with the incident frequencies and satisfy the frequency-matching condition \[41\]. Specifically, assuming incident light at \(\omega_0\) and \(\omega_m\), it follows by inspection of Eqs. (1) to (4) that preshifting the linear cavity resonances away from the incident frequencies according to the transformation
\[
\omega_{0}^{\text{crit}} = \omega_0 \frac{1 - \alpha_0 |d_0^{\text{crit}}|^2 - \alpha_{0m} |d_m^{\text{crit}}|^2 - \alpha_{0p} |d_p^{\text{crit}}|^2}{\omega_m},
\]
\[
\omega_{m}^{\text{crit}} = \omega_m \frac{1 - \alpha_m |d_0^{\text{crit}}|^2 - \alpha_{mm} |d_m^{\text{crit}}|^2 - \alpha_{mp} |d_p^{\text{crit}}|^2}{\omega_p},
\]
\[
\omega_{p}^{\text{crit}} = \omega_p \frac{2\omega_0 - \omega_m}{\omega_p} \frac{1 - \alpha_p |d_0^{\text{crit}}|^2 - \alpha_{pm} |d_m^{\text{crit}}|^2 - \alpha_{pp} |d_p^{\text{crit}}|^2}{\omega_p},
\]
yields the same steady-state critical solution obtained for \(\alpha = 0\), where \(d^{\text{crit}}\) denotes the critical, steady-state cavity fields.

An alternative approach to excite the critical solution above in the presence of SPM and XPM is to detune the incident frequencies away from \(\omega_0\) and \(\omega_m\), keeping the two cavity frequencies unchanged, while preshifting \(\omega_p\) to enforce frequency matching. Specifically, by inspection of Eqs. (12) to (14), it follows that choosing input-light frequencies
\[
\omega_{0}^{\text{crit}} = \omega_0(1 - \alpha_0 |d_0^{\text{crit}}|^2 - \alpha_{0m} |d_m^{\text{crit}}|^2 - \alpha_{0p} |d_p^{\text{crit}}|^2) ,
\]
\[
\omega_{m}^{\text{crit}} = \omega_m(1 - \alpha_m |d_0^{\text{crit}}|^2 - \alpha_{mm} |d_m^{\text{crit}}|^2 - \alpha_{mp} |d_p^{\text{crit}}|^2) ,
\]
and tuning \(\omega_p\) such that
\[
\omega_{p}^{\text{crit}} = \omega_0(1 - \sum \alpha_0 |d_0^{\text{crit}}|^2 - \omega_m (1 - \sum \alpha_m |d_m^{\text{crit}}|^2) - \sum \alpha_m |d_m^{\text{crit}}|^2 - \omega_p |d_p^{\text{crit}}|^2) ,
\]
yields the same steady-state critical solution above. This approach is advantageous in that the requirement that all three cavity frequencies be simultaneously and independently tuned (postfabrication) is removed in favor of tuning a single cavity mode. Given a scheme to tune the frequencies of the cavity modes that achieves perfect frequency matching at the critical power, what remains is to analyze the stability and excitability of the new critical solution, which can be performed using a straightforward linear stability analysis of the coupled-mode equations \[38\]. Before addressing these questions, however, it is important to address a more serious concern.

C. Frequency mismatch

Regardless of the tuning mechanism, in practice one can never fully satisfy perfect frequency matching (even when SPM and XPM can be neglected) due to fabrication imperfections. In general, one would expect the finite bandwidth to
mean that there is some tolerance $\sim 1/Q_p$ on any frequency mismatch $\Delta \omega = 2 \omega_0 - \omega_{cm} - \omega_p \lesssim \omega_p/Q_p$ [60]. However, here we find that instabilities and strong modifications of the cavity line shapes arising from the particular nature of this nonlinear process lead to extreme, subbandwidth sensitivity to frequency deviations that must be carefully examined if one is to achieve high-efficiency operation.

To illustrate the effects of frequency mismatch, we first consider an ideal, lossless system with zero SPM and XPM ($\alpha = 0$) and with incident light at frequencies $\omega_0 = \omega_{cm}$, and with powers $P_0^{\text{crit}}$ and $P_m$, respectively. With the exception of $\alpha$, the coupling coefficients and cavity parameters correspond to those of the 2D design described in Sec. III A. Figure 3 (top) shows the steady-state conversion efficiency $\eta$ (solid lines) as a function of the frequency mismatch $\Delta \omega_p = \omega_{cm} - \omega_p$ away from perfect frequency matching, for multiple values of $P_m = [0.001, 0.01, 0.1] P_0^{\text{crit}}$, with dark gray (blue) and light gray (red) solid lines denoting stable and unstable steady-state fixed points. As shown, solutions come in pairs of stable and unstable fixed points, with the stable solution approaching the maximum efficiency $\eta^{\text{max}}$ critical solution as $P_m \rightarrow 0$. Moreover, one observes that as $\Delta \omega_p$ increases for finite $P_m$, the stable and unstable fixed points approach and annihilate one other, with limit cycles appearing in their stead (an example of what is known as a “saddle-node homoclinic bifurcation” [69]). We stress that these bifurcations differ from the conventional Hopf bifurcations observed in optical parametric oscillators [70,71]. In a Hopf bifurcation, limit cycles are born when a fixed point becomes unstable, and are therefore associated with the presence of one or more unstable fixed points. In contrast, the limit cycles obtained here are not associated with any particular fixed points, but arise because two fixed points, one stable and the other unstable, annihilate each other at the onset of the bifurcation, a so-called saddle-node bifurcation. The limit cycle is therefore the remnant of the homoclinic orbit that connected the two fixed points, a so-called “saddle node-homoclinic bifurcation.”

The frequency mismatch at which this bifurcation occurs is proportional to $P_m$, so that, as $P_m \rightarrow 0$, the regime over which there exist high-efficiency steady states reduces to a single fixed point occurring at $\Delta \omega_p = 0$. Beyond this bifurcation point, the system enters a limit-cycle regime (shaded regions) characterized by periodic modulations of the output signal in time [37,38,72]. Interestingly, we find that the average efficiency of the limit cycles (dashed lines)

$$\bar{\eta} = \lim_{T \to \infty} \frac{1}{T} \int_0^T dt \eta(t),$$

remains large $\sim \eta^{\text{max}}$ even when $\Delta \omega_p$ is several fractional bandwidths. The inset of Fig. 3 (top) shows the efficiency of this system as a function of time (in units of the lifetime $\tau_0$) for large mismatch $\Delta \omega_p = 3 \omega_p^{\text{crit}}/2 Q_p$. As expected, the modulation amplitude and period of the limit cycles depend on the input power and mismatch, and in particular we find that the amplitude goes to zero and the period diverges $\sim 1/\Delta \omega_p$ as $\Delta \omega_p \to 0$. This behavior is observed across a wide range of $P_m$, with larger $P_m$ leading to lower $\bar{\eta}$ and larger amplitudes. For small-enough mismatch, the modulation frequency enters the THz regime, in which case standard...
rectifications procedures [73] can be applied to extract the useful THz oscillations [4,5,74–77].

Frequency mismatch leads to similar effects for finite \( \alpha \), including homoclinic bifurcations and corresponding high-efficiency limit cycles that persist even for exceedingly large frequency mismatch. One important difference, however, is that the redshift associated with SPM and XPM creates a strongly asymmetrical lineshape that prevents high-efficiency operation for \( \Delta \omega < 0 \). Figure 3 (bottom) shows the stable and unstable fixed points (solid lines) and limit cycles (dashed regions) as a function of \( \Delta \omega \), for the same system of Fig. 3 (top) but with finite \( \alpha \) and for two values of \( P_m = \{0.001, 0.01\} P^\text{crit}_m \). As before, the coupling coefficients and cavity parameters correspond to those of the 2D design described in Sec. III A. Here, in contrast to the \( \alpha = 0 \) case, the critical incident frequencies \( \omega^0_{\text{cm}} \) and \( \omega^0_{\text{cp}} \) are generally different from \( \omega_{\text{cm}} \) and \( \omega_{\text{cp}} \). Aside from the asymmetrical lineshape, one important difference from the \( \alpha = 0 \) case is the presence of additional stable and unstable low-efficiency solutions. Multistability complicates matters since, depending on the initial conditions, the system can fall into different stable solutions and in particular, simply turning on the source at the critical input power may result in an undesirable low-efficiency solution. One well-known technique that allows such a system to lock into the desired high-efficiency solutions is to superimpose a gradual exponential turn-on of the pump with a Gaussian pulse of larger amplitude [37]. We found that a single Gaussian pulse with a peak power of \( 4 P_0 \) and a temporal width \( \sim \tau_m \), depicted in the right inset of Fig. 3 (bottom), is sufficient to excite high-efficiency limit cycles in the regime \( \Delta \omega > 0 \).

Despite their high efficiencies (even for large \( \Delta \omega \gtrsim 1 \)), the limit-cycle solutions above leave something to be desired. Depending on the application, it may be desirable to operate at high-efficiency fixed points. One way to achieve this for nonzero frequency mismatch is to abandon the critical solution and instead choose incidence parameters that exploit SPM and XPM to enforce perfect frequency matching and 100% depletion of the pump, i.e.,

\[
\omega^\text{NL}_{\text{cp}} + \omega^\text{NL}_{\text{cm}} = 2 \omega^\text{NL}_{\text{cp}},
\]

\[
s_0 = 0.0.
\]

Specifically, enforcing Eqs. (19) and (20) by solving Eqs. (1) to (4) for \( \omega_{\text{dep}}^0, \omega_{\text{cm}}^0, P_{\text{dep}}^0 \), and \( P_{\text{dep}}^m \), we obtain a depleted steady-state solution \( \omega_k^\text{dep} \) that, in contrast to the critical solution \( \omega_k^\text{crit} \), yields a steady-state efficiency that corresponds to 100% depletion of the pump regardless of frequency mismatch. Note that we are not explicitly maximizing the conversion efficiency, but rather enforcing complete conversion of pump energy in the presence of frequency mismatch, at the expense of a nonnegligible input \( P_m^\text{dep} \). Figure 4 shows the depleted steady-state efficiency \( \eta_0^\text{dep} \) (solid line) and corresponding incident powers (solid circles and dashed line) as a function of \( \Delta \omega \), for the same system of Fig. 3 (bottom). We find that for most parameters of interest, depleted efficiencies and powers are uniquely determined by Eqs. (19) and (20). As expected, the optimal efficiency occurs at \( \Delta \omega = 0 \) and corresponds to the critical solution, so that \( P_{\text{dep}}^0 = P_{\text{crit}}^0, P_{\text{dep}}^m = P_{\text{crit}}^m = 0 \), and \( \eta_0^\text{dep} = \eta^\text{max} \). For finite \( \Delta \omega \neq 0 \), the optimal efficiencies are lower due to the finite \( P_{\text{dep}}^m \), but there exists a broad range of \( \Delta \omega \) over which one obtains relatively high efficiencies \( \sim \eta^\text{max} \). Power requirements \( P_{\text{dep}}^0 \) and \( P_{\text{dep}}^m \) follow different trends depending on the sign of \( \Delta \omega \). Away from zero detuning, \( P_{\text{dep}}^m \) can only increase, whereas \( P_{\text{dep}}^0 \) decreases for \( \Delta \omega < 0 \) and increases for \( \Delta \omega > 0 \). In the latter case, the total input power exceeds \( P_{\text{crit}}^m \) leading to the observed instability of the fixed-point solutions.

Finally, we point out that limit cycles and depleted steady states reside in roughly complementary regimes. Although no stable high-efficiency fixed points can be found in the \( \Delta \omega > 0 \) regime, it is nevertheless possible to excite high-efficiency limit cycles. Conversely, although no such limit cycles exist for \( \Delta \omega < 0 \), it is possible in that case to excite high-efficiency depleted steady states.

### III. FDTD SIMULATIONS AND NANOBEBAM DESIGNS

In this section, we consider concrete and realistic cavity designs in two and three dimensions, and validate the predictions of our TCMT by performing exact nonlinear FDTD simulations in two dimensions. We show that by choosing slightly different designs, one can explore high-efficiency conversion in either the limit-cycle or depleted steady-state regimes. Our designs are based on a particular class of PhC nanobeam structures, depicted schematically in Figs. 5 and 2, where a cavity is formed by the introduction of a defect in a lattice of air holes in dielectric, and coupled to...
Finally, we require that our system supports a single input or output port for light to couple in or out of the cavity, with coupling lifetimes $Q_{sk} \ll Q_{rk}$ to have negligible radiation losses.

### A. 2D design

To explore both high-efficiency limit-cycle and steady-state behaviors, we consider two separate 2D cavity designs, each resulting in different frequency mismatch but similar lifetimes and coupling coefficients. (Note that by “2D” we mean that electromagnetic fields are taken to be uniform in the $z$ direction.) The two cavities follow the same backbone design shown in Fig. 5 which supports three TE-polarized modes ($\mathbf{H} \cdot \hat{z} = 0$) with radiative lifetimes $Q_{sk}^{\text{rad}} = 6 \times 10^4$, $Q_{rk}^{\text{rad}} = 6 \times 10^4$, and $Q_{sk}^{\text{rad}} \approx Q_{rk}^{\text{rad}} = 3 \times 10^3$, and total lifetimes $Q_{sk} = 1200$, $Q_{rk} = 1100$, and $Q_{pp} = 700$, respectively. The nonlinear coupling coefficients are calculated from the linear modal profiles (shown on the inset of Fig. 5) via Eqs. (8) and (7), and are given by

$$\beta = (23.69 + 5.84i) \times 10^{-5} \left( \frac{\chi^{(3)}}{\epsilon_0 a^2 h} \right),$$

$$\alpha_{00} = 4.935 \times 10^{-4} \left( \frac{\chi^{(3)}}{\epsilon_0 a^2 h} \right), \quad \alpha_{mm} = 5.096 \times 10^{-4} \left( \frac{\chi^{(3)}}{\epsilon_0 a^2 h} \right),$$

$$\alpha_{pp} = 4.593 \times 10^{-4} \left( \frac{\chi^{(3)}}{\epsilon_0 a^2 h} \right), \quad \alpha_{0m} = 6.540 \times 10^{-4} \left( \frac{\chi^{(3)}}{\epsilon_0 a^2 h} \right),$$

$$\alpha_{0p} = 5.704 \times 10^{-4} \left( \frac{\chi^{(3)}}{\epsilon_0 a^2 h} \right), \quad \alpha_{pp} = 5.616 \times 10^{-4} \left( \frac{\chi^{(3)}}{\epsilon_0 a^2 h} \right),$$

where the additional factor of $h$ allows comparison to the realistic 3D structure below and accounts for finite nanobeam thickness (again, assuming uniform fields in the $z$ direction).

Compared to the optimal $\beta_{\text{max}} = \frac{1}{4 \sqrt{\epsilon_{\text{air}}} \left( \frac{\omega_0}{c} \right)}$, corresponding to modes with uniform fields inside and zero fields outside the cavity, we find that $\beta = 5.5 \times 10^{-3} \beta_{\text{max}}$ is significantly smaller due to the fact that these TE modes are largely concentrated in air. In the 3D design section below, we choose modes with peaks in the dielectric regions, which leads to much larger $\beta_{\text{max}} = 0.4$. 

To arrive at this 2D design, we explored a wide range of defect parameters, with the defect formed by modifying the radii of a finite set of holes in an otherwise periodic lattice of air holes of period $a$ and radius $R = 0.36a$ in a...
dielectric nanobeam of width $w = 1.2a$ and index of refraction $n = 3.4$. The defect was parametrized via an exponential adiabatic taper of the air-hole radii $r$, in accordance with the formula $r(x) = R(1 - \frac{1}{3}e^{-x/a^2})$, where the parameter $d$ is an “effective cavity length.” Such an adiabatic taper is chosen to reduce radiation and scattering losses at the interfaces of the cavity [80]. Removing holes on one side of the defect couples light to a waveguide with decay rate $\sim 1/\bar{Q}_a$ determined by the number of holes removed [81–83].

### 1. Limit cycles

In this section, we consider a design supporting high-efficiency limit cycles. Choosing $R_0 = 0.149a$, we obtain critical parameters $\omega_{0\text{crit}}^\text{c} = 0.2319(\frac{2\pi\epsilon}{a})$, $\omega_{m\text{crit}}^\text{c} = 0.2121(\frac{2\pi\epsilon}{a})$, $\omega_{p\text{crit}} = 0.2530(\frac{2\pi\epsilon}{a})$, and $P_{0\text{crit}} = 10^{-3}(\frac{2\pi\epsilon n_0 h}{a^3})$, corresponding to frequency mismatch $\Delta_0 \approx 3\omega_{0\text{crit}}^\text{c}/2Q_a$ and critical efficiency $\eta_{\text{max}} \approx 0.51$. Choosing a small but finite $P_m = 0.01P_{0\text{crit}}$, it follows from Fig. 3 (dashed line) that the system will support limit cycles with average efficiencies $\bar{\eta} \approx 0.65\eta_{\text{max}}$. To excite these solutions, we employed the priming technique described in Sec. II C. Figure 6 shows $\bar{\eta}$ as a function of $P_0$, for incident frequencies $\omega_0 = \omega_{0\text{crit}}^\text{c}$ determined by Eqs. (15) and (16), as computed by our TCMT (dotted gray line) as well as by fully vectorial nonlinear FDTD simulations (solid circles). The two show excellent agreement. For $0.7 < P_0/P_{0\text{crit}} < 3$, we observe limit cycles with relatively high $\bar{\eta}$, in accordance with the TCMT predictions, whereas outside of this regime, we find that the system invariably falls into low-efficiency fixed points. The periodic modulation of the limit cycles means that instead of a single peak, the spectrum of the output signal consists of equally spaced Fourier peaks that decrease in magnitude away from $\omega_{p\text{crit}}$. The top and bottom insets of Fig. 6 show the corresponding frequency spectra of the TCMT and FDTD output signals around $\omega_{p\text{crit}}$, for a particular choice of $P_0 \approx P_{0\text{crit}}$ [light gray (red) circle], showing agreement both in the relative magnitude and spacing $\approx 2.5 \times 10^{-3}(\frac{2\pi\epsilon}{a})$ of the peaks.

### 2. Depleted steady states

In this section, we consider a design supporting high-efficiency, depleted steady states. Choosing $R_0 = 0.143a$, one obtains critical parameters $\omega_{0\text{crit}} = 0.2320(\frac{2\pi\epsilon}{a})$, $\omega_{m\text{crit}}^\text{c} = 0.2118(\frac{2\pi\epsilon}{a})$, $\omega_{p\text{crit}} \approx 0.2532(\frac{2\pi\epsilon}{a})$, and $P_{0\text{crit}} = 10^{-3}(\frac{2\pi\epsilon n_0 h}{a^3})$, corresponding to frequency mismatch $\Delta_0 \approx -0.60\omega_{0\text{crit}}^\text{c}/2Q_a$ and critical efficiency $\eta_{\text{max}} \approx 0.51$. Choosing incident frequencies $\omega_0 = 0.2320(\frac{2\pi\epsilon}{a})$, $\omega_m = 0.2119(\frac{2\pi\epsilon}{a})$, and incident powers $P_0 = 0.7P_{0\text{crit}}$ and $P_m = 0.04P_{0\text{crit}}$, it follows from Fig. 4 (dashed line) that the system supports stable, depleted steady states with efficiencies $\approx 0.95\eta_{\text{max}}$. Figure 7 shows the spectral profile (in arbitrary units) of the system, showing full depletion of the pump [dark gray (blue)] and correspondingly high conversion of the signal and idler frequencies [light gray (red)]. For $P_0 \gtrsim 0.8P_{0\text{crit}}$, the system becomes ultrasensitive to the priming parameters, in which case high-efficiency solutions can only be excited by adiabatic tuning of the pump power (see text).

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**FIG. 7.** (Color online) Conversion efficiency $\eta$ (normalized by the maximum achievable efficiency $\eta_{\text{max}}$) of depleted states as a function of power $P_0$ (normalized by $P_{0\text{crit}}$), at incident frequencies $\omega_0^\text{dep}$ and $\omega_m^\text{dep}$, and a fixed power $P_m^\text{dep} \approx 0.2P_{0\text{crit}}$. The modal parameters are obtained from the 2D cavity of Fig. 5, with $R_0 = 0.143a$ leading to a detuning $\Delta_0 \approx -0.60\omega_{0\text{crit}}^\text{c}/2Q_a$, corresponding to the dashed line in Fig. 3 (bottom). Solid circles and dotted gray lines denote results as computed by FDTD and TCMT. Insets show the spectra of the output light for a given $P_0$ [light gray (red) circle], and for both FDTD and TCMT.
shows the efficiency of the system as a function $P_0$, with all other incident parameters fixed to the depleted-solution values above, where dark gray (blue) and light gray (red) lines denote stable and unstable solutions, respectively. As before, we employ the priming technique of Sec. IIIC to excite the desired high-efficiency solutions and obtain excellent agreement between the TCMT (dotted gray line) and FDTD simulations (solid circles). Exciting the high-efficiency solutions by steady-state input “primed” with a Gaussian pulse is convenient in FDTD because it leads to relatively short simulations, but is problematic for other incident parameters fixed to the depleted-solution realization. The cavity supports three TE00 modes (depicted in Fig. 2, as a feasible candidate for experimental realization. The cavity defect is induced via a linear taper of $a_i$ over a chosen set of $2\bar{N}$ segments, according to the formula

$$a_i = a \left( f_a + \frac{N - 1}{N} |i| - 1 \right) , \quad |i| \leq \bar{N}$$

$$= a , \quad |i| > \bar{N} .$$

To arrive at our particular design, we chose $f_a = 0.85, N = 21, \bar{N} = 9$ and varied the central cavity length $L$ to obtain the desired TE00 modes. Assuming total modal lifetimes $Q_0 = 8500, Q_m = 3000$, and $Q_p = 3000$ using these design parameters, we obtain critical parameters $\alpha_0^{\text{crit}} = 0.2843(\frac{2\pi c}{a}), \alpha_m^{\text{crit}} = 0.2798(\frac{2\pi c}{a}), \alpha_p^{\text{crit}} = 0.2895(\frac{2\pi c}{a})$, and $P_0^{\text{crit}} = 5 \times 10^{-5}(\frac{2\pi c a^2}{\mu_0})$, corresponding to frequency mismatch $\Delta_c \approx -0.07\alpha_0^{\text{crit}}/(2Q_p)$ and $n_{\text{max}} = 0.42$. Note that because the radiative losses in this system are nonnegligible, the maximum efficiency of this system is $\approx 82\%$ of the optimal achievable efficiency $=\omega_p/(2\omega_m) \approx 0.51$. At these small $\Delta_c$, we find that depletion of the pump is readily achieved through the critical parameters associated with perfect frequency matching. However, as illustrated in Sec. IIIA 1, one can also choose a design that supports high-efficiency limit cycles.

### 1. Power requirements

Thus far, we have expressed the power requirements of this system in dimensionless units of $2\pi c e_0 a^2/\chi (3)$. Choosing to operate at telecom wavelengths $\lambda_c \equiv 2\pi c/\omega_c = 1.5 \mu m$, with corresponding $n \approx 3.4$ and $\chi (3) = 2.8 \times 10^{-18} m^2/V^2$ [1], we find that $a = 0.2848 \times 1500 = 427 \mu m$ and $P_0^{\text{crit}} \approx 50 mW$. We note, however, that although our analysis above incorporates effects arising from linear losses (e.g., due to material absorption or radiation), it neglects important and detrimental sources of nonlinear losses in the telecom range, including two-photon and free-carrier absorption [86,87]. Techniques that mitigate the latter exist, e.g., reverse biasing [88], but in their absence it may be safer to operate in the spectral region below the half-band-gap of Si [78]. One possibility is to operate at $\lambda_c = 2.2 \mu m$, where $\chi (3) \approx 1.5 \times 10^{-10} m^2/V^2$ [78], leading to $a = 627 \mu m$, and approximately four-times larger $P_0^{\text{crit}} \approx 200 mW$. For a more detailed analysis of nonlinear absorption in triply resonant systems, the reader is referred to Ref. [89]. While that work does not consider the effects of nonlinear dispersion, SPM, and XPM, or frequency mismatch, it does provide upper bounds on the maximum efficiency in the presence of two-photon and free-carrier absorption.

### IV. CONCLUDING REMARKS

In conclusion, by combining TCMT with fully nonlinear FDTD simulations, we have demonstrated the possibility of achieving highly efficient DFWM at low input powers ($\approx 50 mW$) and large bandwidths ($Q \sim 1000$) in a realistic and chip-scale ([$\mu m$]) nanophotonic platform (silicon nanobeam cavity). Our theoretical analysis extends the initial work of the authors of Ref. [41] by incorporating and analyzing important effects arising from linear losses, SPM and XPM,
as well as mismatch of the cavity-mode frequencies, e.g., such as those that arise from fabrication imperfections, where the latter was shown to lead to a variety of interesting dynamical behaviors, including limit cycles that arise in the presence of infinitesimally small frequency mismatch near critical solutions. Although power requirements in the tens of mWs are not often encountered in conventional chip-scale Si nanophotonics, they are comparable if not smaller than those employed in conventional centimeter-scale DFWM schemes [88,90,91]. Our proof-of-concept design demonstrates that full cavity-based DFWM not only reduces device dimensions down to μm scales, but also allows depletion of the pump with efficiencies close to unity. Compared to conventional integrated whispering-gallery-mode (WGM) resonators [22,92,93], nanobeam cavities offer much smaller mode volumes, ~(λ/2)^3 in nanobeams as compared to ~100(λ/2)^3 in WGM cavities, and therefore allow exploration of these processes at low powers and much larger bandwidths (which is especially important in this system due to its sensitivity to frequency mismatch). From a fabrication viewpoint, they are also desirable in that they allow for minimal footprint and maximal device density on chip. Finally, we emphasize that there is considerable room for additional design optimization. For instance, we find that increasing the radiative lifetimes of processes at low powers and much larger bandwidths (which is especially important in this system due to its sensitivity to frequency mismatch). From a fabrication viewpoint, they are also desirable in that they allow for minimal footprint and maximal device density on chip. Finally, we emphasize that there is considerable room for additional design optimization. For instance, we find that increasing the radiative lifetimes of

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