Theoretical Framework for the "Reconfigurable SHG in Si_3N_4 Microrings via Self-Injection Locking and All-Optical Poling: A Design Study"

B. E. Castiblanco

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1 Introduction

Nonlinear integrated photonics in silicon nitride (SiN) waveguides and resonators has attracted significant attention due to the wide transparency window, low propagation loss and CMOS compatibility of SiN platforms. While SiN is intrinsically centro-symmetric and thus lacks a bulk second-order susceptibility $\chi^{(2)}$, effective $\chi^{(2)}$ responses can be engineered via surface symmetry breaking, strain, or more recently via all-optical poling (AOP) based on the coherent photogalvanic effect. In AOP, simultaneous excitation of a waveguide or resonator at the fundamental harmonic (FH) and second harmonic (SH) frequencies leads to a spatially modulated space-charge field, which in turn induces a quasi-phase-matching (QPM) $\chi^{(2)}$ grating through an effective third-order process (EFISH).

In parallel, self-injection locking (SIL) of semiconductor lasers to high-Q microresonators allows large reductions in laser linewidth and frequency stabilization without electronic feedback. Combining SIL, AOP, and second-harmonic generation (SHG) in SiN microrings offers a powerful route to compact, integrated visible-frequency sources and frequency combs.

The aim of this design study is to:

(i) connect straight-waveguide modal simulations (EMode) of SiN/SiO_2 structures to the effective propagation constants and dispersion of a SiN microring resonator,

(ii) compute the phase mismatch $\Delta k(\lambda)$ and QPM period $\Lambda(\lambda)$ relevant for SHG between FH and SH modes,

(iii) embed these quantities into models of AOP and SHG in a doubly resonant microring, and

(iv) explore numerically how quasi-phase matching via AOP modifies SHG conversion efficiency as a function of input power.

We proceed step by step, introducing the required equations and then showing how each piece is implemented in Python, with code snippets collected and commented in the appendix.

2 Waveguide Modes and Propagation Constants

2.1 Straight waveguide approximation for the microring

We consider a SiN waveguide with a rectangular (or trapezoidal) core of width w_{core} and height h_{core}, embedded in SiO_2 (BOX and top cladding). The microring resonator is formed by bending this waveguide into a ring of radius $R = 900\,\mu\text{m}$. For such a large radius, bending-induced perturbations of the fundamental TE mode profile and effective index are negligible, and the microring modes can be accurately approximated by the straight waveguide modes.

Thus, for each wavelength λ we obtain from EMode:

- the effective index of the FH mode $n_{\mathrm{eff},\omega}(\lambda)$ in the C-band (e.g. 1520 nm–1600 nm),
- the effective index of the corresponding SH mode $n_{\mathrm{eff},2\omega}(\lambda/2)$ near 775 nm.

2.2 Propagation constants

The propagation constant of a mode is

$$\beta(\lambda) = \frac{2\pi}{\lambda} n_{\mathrm{eff}}(\lambda). \tag{1}$$

For the FH and SH modes we write

$$\beta_\omega(\lambda_\omega) = \frac{2\pi}{\lambda_\omega} n_{\mathrm{eff},\omega}(\lambda_\omega), \tag{2a}$$

$$\beta_{2\omega}(\lambda_{2\omega}) = \frac{2\pi}{\lambda_{2\omega}} n_{\mathrm{eff},2\omega}(\lambda_{2\omega}), \tag{2b}$$

where $\lambda_{2\omega} = \lambda_\omega/2$ for SHG.

2.3 Group index and dispersion

The group index is defined as

$$n_g(\lambda) = n_{\mathrm{eff}}(\lambda) - \lambda \frac{dn_{\mathrm{eff}}}{d\lambda}, \tag{3}$$

which captures the wavelength dependence of n_{eff}. The derivative is computed numerically from the EMode data via finite differences.

In the microring, the free spectral range (FSR) at a given wavelength is

$$\mathrm{FSR}(\lambda) = \frac{c}{n_g(\lambda) L}, \tag{4}$$

with $L = 2\pi R$ the ring circumference and c the speed of light. Separate FSRs for FH and SH are obtained from their respective group indices.

3 Phase Mismatch and Quasi-Phase Matching

3.1 Phase mismatch for SHG

For second-harmonic generation (SHG) in a waveguide or resonator, the phase-matching condition for efficient energy transfer from FH to SH is

$$2\beta_\omega = \beta_{2\omega}. \tag{5}$$

In general this is not exactly satisfied, so we define the phase mismatch

$$\Delta k(\lambda_\omega) = \beta_{2\omega}(\lambda_\omega/2) - 2\,\beta_\omega(\lambda_\omega). \tag{6}$$

Using Eq. (2a) and Eq. (2b), this can be computed directly from the EMode-extracted effective indices. In SiN waveguides, due to stronger confinement and slightly higher material index at the SH wavelength, $n_{\mathrm{eff},2\omega}(\lambda/2)$ tends to be sufficiently larger than $n_{\mathrm{eff},\omega}(\lambda)$ so that $\Delta k \neq 0$ and natural phase matching is not available.

In the notebook, Eq. (6) is implemented in the modal data block and stored as the array `delta_k`.

3.2 Coherence length and QPM period

The coherence length of the FH–SH interaction is defined as

$$L_c = \frac{\pi}{|\Delta k|}, \tag{7}$$

which is the distance over which FH and SH accumulate a relative phase of π.

Quasi-phase matching (QPM) circumvents the lack of exact phase matching by periodically *modulating the sign or magnitude* of the effective nonlinearity $\chi^{(2)}$ with a spatial period Λ, such that the generated SH field experiences a net constructive contribution over many periods. For first-order QPM, the optimal period is

$$\Lambda = \frac{2\pi}{|\Delta k|} = 2L_c. \tag{8}$$

Thus, once $\Delta k(\lambda)$ is known from Eq. (6), the required QPM period $\Lambda(\lambda)$ for each FH wavelength follows immediately.

In the EMode-based analysis, the QPM period is computed via Eq. (8) and plotted versus the FH wavelength.

3.3 Mismatch factor for SHG efficiency

Even with a uniform $\chi^{(2)}$ and no explicit QPM, it is useful to quantify how severely phase mismatch suppresses SHG. For an interaction length L, the effective contribution of the nonlinear polarization is modulated by a factor

$$\mathrm{sinc}\left(\frac{\Delta k L}{2}\right) = \frac{\sin\left(\Delta k L/2\right)}{\Delta k L/2}, \tag{9}$$

which enters the SHG efficiency as a multiplicative factor. When the microring length L and Δk are known, this factor quantifies the degree of phase mismatch. In our coupled-mode model we incorporate Eq. (9) via a *mismatch factor* that rescales the nonlinear coupling coefficient.

4 Ring Resonator Model

4.1 Resonance condition

For a microring of circumference $L = 2\pi R$, the resonance condition for a given mode is

$$m\lambda = n_{\mathrm{eff}}(\lambda)L \tag{10}$$

$$n_{\mathrm{eff}}(T) = n_{\mathrm{eff}}(T_0) + \frac{dn}{dT}(T - T_0) \tag{11}$$

where m is an integer azimuthal mode number. When the waveguide dispersion $n_{\mathrm{eff}}(\lambda)$ is known from EMode, Eq. (10) can be solved (at least approximately) for the resonant wavelengths.

At the FH, the ring supports resonances near $\lambda_\omega \approx 1550\,\mathrm{nm}$, and at the SH near $\lambda_{2\omega} \approx 775\,\mathrm{nm}$. Double resonance arises when both FH and SH simultaneously satisfy Eq. (10) for some pair $(m_\omega, m_{2\omega})$ within a given detuning tolerance.

4.2 Quality factors and decay rates

Each resonance is characterized by a quality factor Q that can be decomposed into intrinsic (Q_{int}) and coupling (Q_{cpl}) contributions,

$$\frac{1}{Q_{\text{loaded}}} = \frac{1}{Q_{\text{int}}} + \frac{1}{Q_{\text{cpl}}}. \tag{12}$$

The (power) decay rate at angular frequency ω is

$$\kappa = \frac{\omega}{Q_{\text{loaded}}}, \tag{13}$$

with intrinsic and coupling components κ_{int} and κ_{ex} defined analogously. These rates are used in the time-domain coupled-mode equations for the intracavity fields.

5 All-Optical Poling (AOP) Model

5.1 Photogalvanic effect and effective $\chi^{(2)}$

AOP in SiN is based on the coherent photogalvanic effect: illumination of the waveguide by FH and SH fields induces a spatially varying photocurrent and subsequent space-charge field $E_{\text{sc}}(z,t)$, which breaks local inversion symmetry and yields an effective second-order nonlinearity via the third-order susceptibility $\chi^{(3)}$ (electric-field-induced second harmonic, EFISH). In a simplified scalar form, the induced $\chi^{(2)}_{\text{eff}}$ is

$$\chi^{(2)}_{\text{eff}}(z,t) = 3\chi^{(3)} E_{\text{sc}}(z,t), \tag{14}$$

$$\Delta k_{\text{eff}} = \Delta k - K_G \tag{15}$$

where $\chi^{(3)}$ is the relevant third-order susceptibility component.

The AOP process leads to a spatial modulation of E_{sc} with the QPM period Λ determined by the interference between FH and SH fields, which is linked to the phase mismatch Δk (Section 3). In the present model we focus on the temporal build-up of the *average* effective field and treat the spatial dependence separately through the mismatch factor.

5.2 Rate equation for the space-charge field

We adopt a phenomenological rate equation for the average space-charge field $E(t)$:

$$\frac{dE}{dt} = A_{\text{CPG}} I_\omega I_{2\omega} - \frac{E}{\tau_{\text{erase}}}, \tag{16}$$

where:

- I_ω and $I_{2\omega}$ are the intracavity intensities at FH and SH, respectively,
- A_{CPG} is an effective photogalvanic gain constant,
- τ_{erase} is the characteristic time for erasure of the poling (e.g. due to dark conductivity or thermal effects).

For a constant pump, Eq. (16) yields an exponential approach to a steady-state field $E_\infty = A_{\text{CPG}} I_\omega I_{2\omega} \tau_{\text{erase}}$.

Combining Eq. (16) with Eq. (14) gives the time-dependent effective $\chi^{(2)}_{\text{eff}}(t)$.

6 Self-Injection Locking (SIL) Model

Self-injection locking arises when narrow-band backscattered light from the resonator is fed back into the laser cavity, effectively providing an optical feedback that can reduce the laser linewidth and stabilize its frequency to a cavity resonance. A simple heuristic description can be obtained from the Adler equation for a driven oscillator.

6.1 Locking range and linewidth narrowing

We denote:

- Q as the cavity quality factor at FH,
- k_{back} as an effective backscatter coefficient,
- $\Delta\nu$ as the laser linewidth.

A heuristic expression for the locking half-range is

$$\Delta\nu_{\text{lock}} \propto k_{\text{back}} Q, \tag{17}$$

and the linewidth narrowing factor can be written as

$$\Delta\nu_{\text{SIL}} \approx \frac{\Delta\nu_0}{1+G}, \qquad G \propto k_{\text{back}} Q, \tag{18}$$

where $\Delta\nu_0$ is the free-running linewidth and G is an effective feedback gain.

In the notebook, Eq. (17) and Eq. (18) are implemented by the functions `sil_locking_range` and `sil_linewidth_narrowing`, which are then used to explore how $\Delta\nu_{\text{SIL}}$ and $\Delta\nu_{\text{lock}}$ scale with Q for a given k_{back}.

7 SHG in a Doubly-Resonant $\chi^{(2)}$ Microring

7.1 Coupled-mode equations

We model the intracavity FH and SH fields by slowly varying complex amplitudes $a(t)$ and $b(t)$, normalized such that $|a|^2$ and $|b|^2$ are proportional to the intracavity powers. The coupled-mode equations for a doubly resonant $\chi^{(2)}$ cavity are

$$\dot{a} = \left(i\Delta_\omega - \frac{\kappa_\omega}{2}\right) a + ig\, ba^* + \sqrt{\kappa_{\omega,\text{ex}}}\, s_{\text{in}}, \tag{19a}$$

$$\dot{b} = \left(i\Delta_{2\omega} - \frac{\kappa_{2\omega}}{2}\right) b + ig\, a^2, \tag{19b}$$

where:

- Δ_ω and $\Delta_{2\omega}$ are the detunings of the FH and SH from their respective cavity resonances,
- κ_ω and $\kappa_{2\omega}$ are the total (intrinsic + coupling) decay rates, defined by Eq. (13),
- $\kappa_{\omega,\text{ex}}$ is the coupling rate to the bus waveguide at FH,
- s_{in} is the FH input field, with $|s_{\text{in}}|^2 = P_{\text{in}}$ the input power,
- g is the effective nonlinear coupling coefficient.

7.2 Nonlinear coupling coefficient and mismatch factor

The coupling coefficient g encodes the overlap between FH and SH modes, the effective $\chi^{(2)}$, and the mode normalization. In general,

$$g \propto \frac{\chi_{\text{eff}}^{(2)}}{\sqrt{A_{\text{eff},\omega}^2 A_{\text{eff},2\omega}}}, \tag{20}$$

where A_{eff} are effective mode areas. In our simplified model we write

$$g = \mathcal{O}\,\chi_{\text{eff}}^{(2)} \cdot \text{sinc}\left(\frac{\Delta k L}{2}\right), \tag{21}$$

where:

- $\mathcal{O}$ is a lumped overlap constant (denoted `overlap_scalar` in the code),
- $\chi_{\text{eff}}^{(2)}$ is obtained from the AOP model (Section 5),
- the $\text{sinc}(\Delta kL/2)$ factor from Eq. (9) accounts for the residual phase mismatch Δk computed from the EMode modes for the given geometry.

In the absence of QPM (no AOP grating), the sinc factor can drastically suppress g and thus the SHG efficiency. When QPM is achieved (AOP writes the appropriate Λ), the effective Δk is reduced towards zero and the sinc factor approaches unity.

In the Python implementation, Eq. (21) is captured by the product

$$g = \texttt{overlap\_scalar} \times \chi_{\text{SI}}^{(2)} \times \texttt{mismatch\_factor},$$

where the `mismatch_factor` is defined from Eq. (9) and the ring length L (see Appendix **??**).

7.3 Output powers and SHG vs. input power

The output powers in the bus waveguide are

$$P_{\omega,\text{out}}(t) = \kappa_{\omega,\text{ex}}|a(t)|^2, \tag{22a}$$

$$P_{2\omega,\text{out}}(t) = \kappa_{2\omega,\text{ex}}|b(t)|^2, \tag{22b}$$

and the steady-state SH output is obtained by taking $t \to \infty$ numerically, i.e. by integrating Eq. (19a)–(19b) for a time t_{end} much longer than the cavity lifetime.

To characterize the scaling of SHG, we sweep the input FH power P_{in} and record the steady-state SH output $P_{2\omega,\text{out}}^{(\text{ss})}$ for two cases:

(a) natural phase mismatch (no explicit QPM), $\text{sinc}(\Delta kL/2) < 1$,

(b) idealized QPM (e.g. AOP has written the correct grating), $\text{sinc}(\Delta kL/2) \approx 1$.

This comparison directly shows the impact of QPM on conversion efficiency for the given SiN geometry.

8 Numerical Workflow and Parameter Choices

The full numerical workflow can be summarized as follows:

(i) Use EMode to compute $n_{\text{eff},\omega}(\lambda)$ and $n_{\text{eff},2\omega}(\lambda/2)$ for the SiN/SiO_2 waveguide geometry of interest in the FH and SH bands. Export these as CSV files.

(ii) Construct a combined `modes.csv` file with columns `lambda_m`, `neff_FH`, `neff_SH`.

(iii) In Python, load `modes.csv`, compute β_{ω}, $\beta_{2\omega}$, and $\Delta k(\lambda)$ according to Eq. (6), and then $\Lambda(\lambda)$ via Eq. (8).

(iv) From $n_{\text{eff}}(\lambda)$ compute $n_g(\lambda)$ using Eq. (3) and obtain FSRs via Eq. (4). This ties the waveguide dispersion to the microring resonance structure.

(v) For a chosen reference wavelength λ_0 (e.g. 1550 nm), interpolate $\Delta k(\lambda_0)$, compute the mismatch factor via Eq. (9), and construct the effective nonlinear coupling coefficient g according to Eq. (21).

(vi) Simulate AOP using the rate equation Eq. (16), obtaining a steady-state $\chi^{(2)}_{\text{eff}}$ through Eq. (14).

(vii) Insert g and the cavity decay rates κ_{ω}, $\kappa_{2\omega}$ (Eq. (13)) into the coupled-mode equations Eq. (19a)–(19b), integrate in time, and compute SH output powers according to Eq. (22b).

(viii) Sweep the input power and compare SHG performance with and without QPM (i.e. with and without the sinc-based mismatch factor).

The specific numerical values of R, Q, thermo-optic coefficients, $\chi^{(3)}$, and the overlap constant $\mathcal{O}$ are chosen to be consistent with experimentally reported SiN microrings and can be adjusted to match a given platform.