Coupled-mode theory for microresonators with quadratic nonlinearity

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We use Maxwell’s equations to derive several models describing the interaction of the multi-mode fundamental field and its second harmonic in a ring microresonator with quadratic nonlinearity and quasi-phase-matching. We demonstrate how multi-mode three-wave mixing sums entering nonlinear polarisation response can be calculated via Fourier transforms of products of the field envelopes. Quasi-phase-matching gratings with arbitrary profiles are incorporated seamlessly into our models. We also introduce several levels of approximations allowing to account for dispersion of nonlinear coefficients and demonstrate how coupled-mode equations can be reduced to the envelope Lugiato-Lefever-like equations with self-steepening terms. An estimate for the \( \chi^{(2)} \) induced cascaded Kerr nonlinearity, in the regime of imperfect phase-matching, puts it above the intrinsic Kerr effect by several orders of magnitude.

I. INTRODUCTION

Third-order, \( \chi^{(3)} \), or Kerr, nonlinearity based frequency conversion, comb generation and soliton formation in high-quality factor microresonators \[1,3\] continue to be a fast-expanding direction of applied and fundamental research in small footprint nonlinear photonics \[4,5\]. Using second-order, \( \chi^{(2)} \), nonlinearity has always existed as an alternative, and often a preferred option, for a variety of nonlinear optics applications \[6,8\]. More than two decades ago Refs. \[4,11\] reported experimental realisations, respectively, in space and time, of theoretical predictions \[12,13\] of solitons due to quadratic nonlinearity, which has led to a surge of research in this area, and that is when a sub-area of the resonator quadratic solitons has been shaped \[6,8\]. Though a viable for the resonator (cavity) solitons experimental setting has not been worked out at that time, basic three-wave mixing scenarios have been studied theoretically using adaptations of the Lugiato-Lefever approach \[14\]. In particular, bright spatial and temporal solitons have been reported for the intra-cavity second-harmonic generation \[15\], degenerate \[16,18\] and non-degenerate \[19\] parametric down-conversion, including effects of different group velocities \[20\].

Ref. \[23,24\] are the landmark papers on using high-quality factor whispering gallery microresonators with quadratic nonlinearity for frequency conversion applications. Foundational work on monolithic \( \chi^{(2)} \) Fabry-Perot resonators has been accomplished back in 90th \[21,22\]. Since then, this area has developed with a gradually accelerating pace, see, e.g., Ref. \[2\] for a few years old review and Refs. \[25,41\] for some of the experimental contributions shaping its current state. There are a few good reasons for this surge of interest. Frequency combs with second harmonic are naturally octave wide and therefore are suitable for direct self-referencing \[22\]. Quadratic nonlinearity is also relatively strong. Even if conversion into the second harmonic is inefficient, i.e., phase matching is not perfect, one still can derive advantages in terms of threshold powers relative to the Kerr combs \[37,38,40,41\]. Modulational instability, i.e., side-band generation, due to \( \chi^{(2)} \) effects happens through a range of both normal and anomalous dispersions \[6\], which comes handy, in particular, for visible and UV ranges, and should help to alleviate some of the design, material and pump laser constrains. Material wise, lithium-niobate (LN) has been extensively used for both integrated and bulk cut microresonator devices, see, e.g., \[4,5,34\] and references there in. LN allows to utilise both birefringence- and quasi- phase matching arrangements. Few other important materials to mention are silicon nitride, SiN, \[25,26,35,44\], aluminium nitride, AlN, \[31,40\], and gallium phosphate, GaP, \[32\], GaAs and AlGaAs \[15,47\].

Regarding recent theory and modelling approaches to \( \chi^{(2)} \) resonators, a significant effort \[48,50\] has been focused on utilising the Ikeda map method \[51,52\] and its reductions to the mean field models to describe frequency conversion in centimetre and larger multi-mirror resonators with LN crystals used as a nonlinear element \[53,55\]. This approach yields a Lugiato-Lefever (LL) model, where an evolution coordinate is a round-trip number, and a dispersion operator is applied in the time domain. Time and frequency are conjugate variables, in this formulation, which means that taking a Fourier transform of the envelope function across the computational domain periodic in time recovers frequency spectrum at a given round-trip.

An alternative to the Ikeda map approach is to use a basis of the resonator modes to find a solution to the boundary value problem for the nonlinear and time-dependent Maxwell equations. This method has flourished after it has been applied to describe frequency comb generation and solitons in Kerr microresonators \[58,60\].

Ref. \[61\] uses an example a bidirectionally pumped Kerr resonator to provide a refreshed outlook on this formulation and includes a literature overview. Coupled mode equations, under quite general assumptions, are formally equivalent to an LL equation \[61\]. This formulation of LL is, however, different from the one derived from the Ikeda map. It uses physical time as an evolution vari-
able and its dispersion operator involves an angular coordinate [59]. Hence, for a given time moment, it deals with a spectrum of mode numbers (momenta) and requires periodicity to be applied in the angular coordinate. Thus, this formulation of LL is naturally connected to the initial and boundary conditions of Maxwell equations. Also, it links directly to the familiar methodology from the quantum mechanics text-books dealing with periodic boundary value problems for Schrödinger equation:

\[ i\hbar \frac{\partial \psi}{\partial t} = -\frac{1}{2} D_2 \frac{\partial^2 \psi}{\partial \theta^2} + U(\theta) \psi, \quad \psi(t, \theta) = \psi(t, \theta + 2\pi) \].

Here, polar angle, \( \theta \), and momentum are the conjugate variables. This approach has an advantage of the transparent interpretation of, e.g., side-band growth, when periodic in space modes grow exponentially in time. Note, that a concern discussed in Ref. [62] related to comparison of the LL vs Ikeda approaches has been alleviated in the follow-up papers [64] and [65], that used, respectively, the coupled-mode and Ikeda map connected formulations of the LL model.

Recently, a derivation of the coupled-mode and LL equations from the Maxwell equations for a ring microresonator with \( \chi^{(2)} \) nonlinearity has been sketched in Ref. [66]. Refs. [40, 41, 68] have also announced coupled-mode formulations. A relying on it (in fact, equivalent to it, see Section 8 below) LL model has been used in [35, 64, 67] to study \( \chi^{(2)} \) combs and solitons, and its comparison with experimental data has been encouraging [68, 40]. Below we present a detailed derivation procedure of the coupled-mode equations from the Maxwell equations with \( \chi^{(2)} \) nonlinearity and subsequently transform them to the envelope LL equations.

One of our aims here is to present a formalism underpinning a variety of models that has been and can be used by the community working on the frequency conversion and combs in \( \chi^{(2)} \) microresonators. Apart from providing methodological background for already advertised models [35, 65, 66], we also go beyond them in several aspects. First, we show how the mode number dependent variations of the nonlinear interaction strength for multimode three-wave mixing can be accounted for with various degrees of accuracy. Second, we formulate coupled-mode equations by treating multimode nonlinear sums pseudo-spectrally. Here we use connections with pseudo-spectral approaches developed for quantum Schrödinger equation [69] and for Kerr microresonators [61, 63, 70]. The pseudo-spectral method provides a route for a seamless and approximation free incorporation of arbitrary quasi-phase-matching grating profiles and allows a user to apply fast-Fourier transform to deal with the multi-mode three-wave mixing nonlinear terms. Finally, we briefly address a problem of the relative strength of \( \chi^{(3)} \) and \( \chi^{(1)} \) effects.

Chapter titles used below are self-explanatory, which makes outlining their content here unnecessary.

II. MAXWELL EQUATIONS AND MODE EXPANSION

Quite generally, Maxwell equations for an electric field component \( \mathbf{E}_\alpha \) in a dispersive, spatially inhomogeneous and nonlinear material read as

\[
\begin{align*}
\varepsilon_{\alpha\alpha}(t, r, \theta, z) \frac{\partial^2 \mathbf{E}_\alpha}{\partial t^2} + \nabla \times \left( \mu_{\alpha\alpha}(t, r, \theta, z) \nabla \times \mathbf{E}_\alpha \right) &= \frac{\partial}{\partial t} \left( \sigma_{\alpha\alpha}(t, r, \theta, z) \mathbf{E}_\alpha \right) + \chi^{(2)}_{\alpha\alpha}(t, r, \theta, z) \mathbf{E}_\alpha \times \mathbf{E}_\alpha, \\
\varepsilon_{\alpha\alpha}(t, r, \theta, z) \frac{\partial \mathbf{E}_\alpha}{\partial t} &= \nabla \times \left( \mu_{\alpha\alpha}(t, r, \theta, z) \nabla \times \mathbf{E}_\alpha \right) - \chi^{(2)}_{\alpha\alpha}(t, r, \theta, z) \mathbf{E}_\alpha \times \mathbf{E}_\alpha.
\end{align*}
\]

Here, \( x, y, z \) are spatial coordinates, and implicit summations over the repeated \( \alpha \) is assumed. The first and second terms in the left hand side of Eq. (2.1a) are gradient of divergence and Laplacian, respectively, \( \varepsilon_{\alpha\alpha} \) is the linear dielectric response varying in space and time, \( t, c \) is the vacuum speed of light.

To introduce a ring microresonator geometry, we proceed by defining \( \theta = [0, 2\pi] \) as the azimuthal coordinate varying along the ring circumference, \( z \) axis is perpendicular to the ring plane, while \( r = \sqrt{x^2 + y^2} \) measures distance from the ring centre. We assume that a microresonator is made of a \( z \)-cut uniaxial crystal and \( \varepsilon_{\alpha\alpha} \) is a diagonal matrix. Time to frequency Fourier transforms of \( \varepsilon_{x,y} \) give the ordinary refractive index, \( n_o \), squared, and the transform of \( \varepsilon_{zz} \) gives the extraordinary index, \( n_e \), squared.

\( N_\alpha \) is the second order nonlinear polarization,

\[
N_\alpha = \chi^{(2)}_{\alpha\alpha\alpha\alpha} \mathbf{E}_\alpha \times \mathbf{E}_\alpha = 2d_{\alpha\alpha\alpha} \mathbf{E}_\alpha \times \mathbf{E}_\alpha,
\]

where \( d_{\alpha\alpha\alpha} \) is a reduced \((3 \times 3)\) tensor of the second order nonlinear susceptibility [71, 72]. Linear, \( N_\alpha = 0 \), modes of the resonator are divided into quasi-ordinarily polarised ones, \( s = o \) ( quasi-TE), and quasi-extraordinarily ones, \( s = e \) ( quasi-TM). Generally, modes of an open microresonator have complex eigenfrequencies and do not form an orthogonal basis. We proceed to disregard these effects and later include loss and pump phenomenologically.

\( \mathbf{E}_\alpha \) will be expressed few lines below as a superposition of the linear microresonator modes

\[
\Theta_{s\alpha}(\theta) \Phi_{js\alpha}(r, z) e^{i j \theta - \omega_{js} t},
\]

\[
\Theta_{s\alpha}(\theta) \Phi_{js\alpha}(r, z) e^{i j \theta - \omega_{js} t},
\]

\[
\Theta_{s\alpha}(\theta) \Phi_{js\alpha}(r, z) e^{i j \theta - \omega_{js} t},
\]

Here \( j \) is an azimuthal mode number or angular momentum, and \( \omega_{js} \) is the corresponding frequency. Linear modes can be calculated either asymptotically as Bessel functions [73] or numerically using, e.g., COMSOL. In either case, they are commonly represented by a vector in the polar basis, while \( \chi^{(2)} \) tensors are readily available in the literature in the Cartesian one. Factorization of the intensity profiles into the \( \theta \) and \( (r, z) \) dependent parts
and an assumption that the ordinary modes are quasi-transverse, i.e., their component tangential to the ring can be neglected relative to the dominant radial one, are the approximations that we make here for the sake of transparency:

$$\Theta_{ox}(\theta) = \cos \theta, \quad \Theta_{oy}(\theta) = \sin \theta, \quad \Theta_{oz}(\theta) = 0, \quad \Phi_{jox} = \Phi_{joy} = \Phi_{jor}(r, z),$$

$$\Theta_{ex}(\theta) = \cos \theta, \quad \Theta_{ey}(\theta) = \sin \theta, \quad \Theta_{ez}(\theta) = 1, \quad \Phi_{jex} = \Phi_{jey}(r, z).$$

(2.4a)

(2.4b)

Here Eqs. (2.4a) and (2.4b) apply, respectively, to the families of the ordinary and extraordinary modes.

Three electric field components $\mathcal{E}_a$ can be expressed via the ordinary and extraordinary fields, $\mathcal{E}_{o,c}$, as

$$\mathcal{E}_x = \cos \theta \mathcal{E}_o,$$

$$\mathcal{E}_y = \sin \theta \mathcal{E}_o,$$

$$\mathcal{E}_z = \mathcal{E}_e,$$

$$\mathcal{E}_s = \sum_{j=j_{\min,s}}^{j_{\max,s}} b_{js} \Phi_{js} B_{js}(t) e^{j\theta - i\omega_{js} t} + c.c.,$$

(2.5a)

(2.5b)

(2.5c)

(2.5d)

where $B_{js}$ are the complex mode amplitudes and $b_{js}$ are the normalisation constants. We choose to normalise linear modes as

$$\max_{r,z} |\Phi_{jx}| = 1,$$

(2.6)

and hence units of $b_{js} B_{js}$ are V/m. Scaling factors $b_{js}$ are defined to measure $|B_{js}|^2$ in Watts:

$$b_{js}^2 = \frac{Z_{\text{vac}}}{S_{j}},$$

(2.7)

where $Z_{\text{vac}} = 1/\varepsilon_{\text{vac}} c = 377$ V$^2$/W is the free space impedance \[71\]. $S_{j}$ is the effective transverse area of $\Phi_{jx} = \Phi_{jx}(r|y=0, z)$. Refractive indices are $n_{s}^{o,e} = \int \mathcal{E}_{xx,zz}(r, \tau = \tau_{0}, z = 0) e^{i\omega_{o,e} \tau} d\tau$, where $\tau_{0}$ is the distance from the resonator axis to the intensity maximum.

Below, we consider in detail an example when the ordinary modes are grouped around $j = M_o$ corresponding to the frequency $\omega_{M_o}$ and the extraordinary ones around $j = M_e$ with $\omega_{M_e}$. If the pump is ordinarily polarised, then $\omega_{M_o} \approx 2\omega_{M_e}$ is its second harmonic. Resonance frequencies of the approximate or extraordinary modes can be approximated as

$$\omega_{js} = \omega_{M_o} + D_{1s}(j_s - M_o) + \frac{1}{27} D_{2s}(j_s - M_o)^2$$

$$+ \frac{1}{25} D_{3s}(j_s - M_o)^3 + \frac{1}{45} D_{4s}(j_s - M_o)^4 + \ldots,$$

(2.8a)

$$j_s = \ldots M_s - 2, M_s - 1, M_s, M_s + 1, M_s + 2, \ldots$$

(2.8b)

$D_{1s}/2\pi$ are the repetition rate parameters equalling the free spectral ranges (FSRs). $D_{2s}$ are the second-order dispersions and $D_{(k>2)s}$ are the higher-order dispersion coefficients. We consider the same number, $N$, of modes around both $M_o$ and $M_e$, and therefore can introduce the same mode number offset parameter $\mu$,

$$\mu = -\frac{1}{2} N + 1, \ldots, 0, \ldots, \frac{1}{2} N,$$

(2.9)

giving

$$\omega_{\mu} = \omega_{0s} + D_{1s}\mu + \frac{1}{27} D_{2s}\mu^2 + \frac{1}{25} D_{3s}\mu^3 + \ldots,$$

(2.10a)

$$\omega_{(j=M_e)s} = \omega_{(j=0)s},$$

(2.10b)

for the ordinary and extraordinary resonances.

### III. COUPLED-MODE EQUATIONS AND CHI-2 TENSOR

Making a substitution $t' = t - \tau$ in Eqs. (2.4b), (2.5b) we then assume that material response is fast so that $B_{js}(t - \tau) \approx B_{js}(t) \approx \tau \partial_{\tau} B_{js} + \ldots$. Neglecting all the 2nd and higher-order time derivatives of $B_{js}$ we find that Eq. (2.1a) transforms to

$$c^2 \partial_{\tau} \partial_{\tau} \mathcal{E}_{o,e} \mathcal{E}_{o,e} - c^2 \partial_{\tau} \partial_{\tau} \mathcal{E}_{o,e} + \omega_{o,e}^2 \mathcal{E}_{o,e} = \int_{-\infty}^{\infty} e^{i\omega_{o,e} \tau} \partial_{\tau} \mathcal{E}_{o,e}(t', \tau_0) d\tau'$$

$$\approx \sum_{j_s} b_{js} \Theta_{s} \Phi_{j} \left( -2i\omega_{js} n_{s}^o \mathcal{E}_{js} e^{i\theta - i\omega_{js} t} \partial_{\tau} B_{js} + c.c. \right) = -\partial_{\tau}^2 N_{o,e}.$$  

(3.1)

Refractive indices $n_{s}^{o,e}$ inside the round bracket approximate $(n_{s}^{o,e} + i\omega_{o,e} \partial_{\omega} n_{s}^{o,e})$ combinations formally emerging there.

Eqs. (3.1), are then projected on the linear modes, Eqs. (2.3), (2.4),

$$i\partial_{\tau} B_{js} = \frac{e^{i\omega_{js} t}}{2\omega_{js} b_{js} n_{s}^o V_{js} \Phi_{j}} \int_{0}^{\infty} \int_{-\infty}^{\infty} d\theta N_{s} b_{js} \Phi_{j} e^{-i\theta}.$$

(3.2)

Here

$$V_{js} = 2\pi \int \Phi_{j}^{2s} r dr dz$$

(3.3)

are the mode volume parameters, and

$$N_{o} = \cos \theta N_{x} + \sin \theta N_{y},$$

(3.4a)

$$N_{e} = N_{z}$$

(3.4b)

are the ordinary and extraordinary nonlinear polarizations.

We choose to consider LiNbO$_3$ crystal as an example. It belongs to the point group 3$m(C_{3v})$, and its nonlinear polarization vector \[71, 72\] is $(N_{x}, N_{y}, N_{z})^T = G(\Theta) \times$

$$2 \begin{bmatrix} 0 & 0 & 0 & 0 & d_{31} & -d_{32} \\ -d_{22} & d_{22} & 0 & d_{31} & 0 & 0 \\ d_{31} & -d_{32} & d_{32} & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \varepsilon_{x}^2 \\ \varepsilon_{y}^2 \\ \varepsilon_{z}^2 \\ 2\varepsilon_{x} \varepsilon_{y} \\ 2\varepsilon_{x} \varepsilon_{z} \\ 2\varepsilon_{y} \varepsilon_{z} \end{bmatrix}.$$
Hence,
\[
N_x = 2G(\theta)\big(2d_{33}E_xE_x - 2d_{22}E_xE_y\big),
\]
\[
N_y = 2G(\theta)\big(-d_{22}E_xE_x + d_{22}E_yE_y + 2d_{31}E_yE_z\big),
\]
\[
N_z = 2G(\theta)\big(d_{31}E_xE_x + d_{31}E_yE_y + d_{33}E_zE_z\big).
\]
(3.6a) (3.6b) (3.6c)

Values of the nonlinear tensor elements are \(d_{22} \approx 2.3 \text{pm/V}, d_{33} \approx 4.8 \text{pm/V}, d_{31} \approx 29.7 \text{pm/V}\). \(G(\theta)\) is a profile of the quasi-phase matching grating [7, 74], see Section 4.

Using Eqs. (2.5a), (2.6) helps to transform Eqs. (3.4)
\[
N_o = 2G(\theta)\big(2d_{33}E_oE_o - d_{22} \sin 3\theta E_o^3\big),
\]
\[
N_e = 2G(\theta)\big(d_{31}E_o^2 + d_{33}E_e^2\big).
\]
(3.7a) (3.7b)

Eqs. (3.2) considered together with Eqs. (3.7), (2.5d) make a self-consistent system of equations, that only miss appropriate pump and loss terms to model a typical frequency conversion experiment in a microresonator. Postponing introducing of the latter saves us a considerable amount of space in Section 5, where we elaborate approximations for Eqs. (3.2), allowing to efficiently handle integration in \(r\) and \(z\), while still accounting for dispersion of nonlinear effects.

**IV. MOMENTUM AND FREQUENCY MATCHING**

The efficiency of frequency conversion from the pump to the desired frequency is dominantly driven by an interplay of the angular momentum matching and linear dispersion. The latter is encoded in \(\omega_{js}\) and becomes important for the multi-mode three-wave mixing, i.e., comb generation. The angular momentum matching is user-adjusted via, e.g., either temperature tuning of birefringence or periodic polling (quasi-phase-matching) [7, 74, 75].

We assume that the quasi-matching grating is a square function with single or multiple periods and oscillating between \(-1\) and \(+1\),
\[
G(\theta) = \sum_{m=-\infty}^{\infty} G_m e^{im\theta},
\]
(4.1a)
\[
\text{max } G_m = G_{\pm 1}, m \in \mathbb{Z}.
\]
(4.1b)

where \(m\) are the momenta of the grating harmonics. \(|m| = g\) provides the leading order momentum matching conditions, with \(2\pi m / |g|\) being the corresponding grating period, see Eq. (3.2) below. \(\text{LiNbO}_3\) can be either quasi-phase-matched or birefringence phase-matched [3]. The latter case has been used, e.g., to achieve recent microresonator comb results in the second harmonic configuration [38, 11].

We consider in details an example when the momentum matching is arranged between the ordinary mode \(j = M_o\) at a lower frequency \(\omega_{jo}\) and the extraordinary mode \(j = M_e\) with \(\omega_{je}\) that matches \(2\omega_{jo}\) either exactly or as close as possible. Taking momentum matching as
\[
M_e = 2M_o + g,
\]
(4.2)
\(g\) has to be chosen to minimize (ideally, to make exactly zero) absolute value of the frequency mismatch, \(\varepsilon\), defined as
\[
\varepsilon = 2\omega_{jo} - \omega_{je}.
\]
(4.3)

recall notational transformation from \(\omega_{js}\) to \(\omega_{j\mu}\) in Eqs. (2.10). Birefringence based momentum matching, i.e., \(G(\theta) = 1, g = 0\), is, obviously, \(M_e = 2M_o\).

The above phase matching considerations, as well as formalism developed here, can also be applied for \(d_{33}\) mediated three-wave mixing processes involving only extraordinary resonances, and for the ordinary resonances interacting via \(d_{22}\), and for any combination of thereof, see Eqs. (3.7).

**V. TENSORS OF NONLINEAR COEFFICIENTS AND FREQUENCY MISMATCHES**

If second harmonic generation from the ordinary to extraordinary modes is frequency and momentum matched, then \(d_{33}\) element is engaged for both \(N_o\) and \(N_e\), and the non-matched, \(d_{22}\) (ordinary to ordinary conversion) and \(d_{33}\) (extraordinary to extraordinary conversion) mediated three-wave mixing processes can be disregarded. So that, Eqs. (3.2) become
\[
i\partial_t B_{jo} = \frac{2e^{i\omega_{jo}t}}{\omega_{jo}b_{jo}n_{jo}^2 V_{jo}} \partial_r^2 \int \int r dr dz \ d\theta \ Ge^{-i\theta} E_o E_o E_o, \]
(5.1a)
\[
i\partial_t B_{je} = \frac{e^{i\omega_{je}t}}{\omega_{je}b_{je}n_{je}^2 V_{je}} \partial_r^2 \int \int r dr dz \ d\theta \ Ge^{-i\theta} E_o E_o E_o. \]
(5.1b)

We then express \(E_o\) via their respective mode expansions, Eqs. (2.5b), and replace \(j\) with \(\mu\), see Eqs. (2.8), (2.9), (2.10), which yields double sum expressions for \(E_o E_o\) and \(E_o^2\),
\[
i\partial_t B_{\mu o} = \frac{2e^{i\omega_{\mu o}t}}{\omega_{\mu o}b_{\mu o}n_{\mu o}^2 V_{\mu o}} \partial_r^2 \int \int r dr dz \ d\theta \ Ge^{-i(\mu+M_o)\theta} \times \sum_{\mu_1,\mu_2} \big(b_{\mu_1 o} \Phi_{\mu_1 o} B_{\mu_1 o} e^{i(\mu_1+M_o)\theta-i\omega_{\mu_1 o}t} + c.c.\big) \times \big(b_{\mu_2 e} \Phi_{\mu_2 e} B_{\mu_2 e} e^{i(-\mu+M_o)\theta-i\omega_{\mu_2 e}t} + c.c.\big), \]
(5.2a)
\[
i\partial_t B_{\mu e} = \frac{e^{i\omega_{\mu e}t}}{\omega_{\mu e}b_{\mu e}n_{\mu e}^2 V_{\mu e}} \partial_r^2 \int \int r dr dz \ d\theta \ Ge^{-i(\mu+M_e)\theta} \times \sum_{\mu_1,\mu_2} \big(b_{\mu_1 o} \Phi_{\mu_1 o} B_{\mu_1 e} e^{i(\mu_1+M_o)\theta-i\omega_{\mu_1 o}t} + c.c.\big) \times \big(b_{\mu_2 o} \Phi_{\mu_2 o} B_{\mu_2 e} e^{i(\mu_2+M_o)\theta-i\omega_{\mu_2 e}t} + c.c.\big). \]
(5.2b)
We recall here, that, $\Phi_{\mu\sigma}$ and $\Phi_{\mu e}$ with the same $\mu$ refer to different $j$, $j = M_o + \mu$ and $j = M_e + \mu$, respectively, see Eqs. (2.8), (2.9). Same applies to all other variables and parameters.

By construction, the extraordinary frequencies cluster around the second harmonics of the ordinary ones and therefore, while opening up the brackets, we account only for the terms oscillating with frequencies $\omega_{\mu2e} - \omega_{\mu1o}$ in Eq. (5.2a) and for $\omega_{\mu2o} + \omega_{\mu1o}$ in Eq. (5.2b), and disregard the rest,

$$i\partial_t B_{\mu o} \simeq - \frac{2 e^{i \omega_{\mu o} t}}{\omega_{\mu o}} b_{\mu o} n_{\mu o}^2 V_{\mu o} \times \int \int \int r d\rho d\zeta \Phi_{\mu o} \int d\theta G_{e}^{c(M_e - 2M_o)} \theta \times \sum_{\mu_1 \mu_2} (\omega_{\mu2e} - \omega_{\mu1o})^2 b_{\mu1o} b_{\mu2e} \Phi_{\mu_1o} \Phi_{\mu_2e} \times B_{\mu_1o} + B_{\mu_2e} e^{i(\omega_{\mu2e} - \omega_{\mu1o})t},$$

(5.3a)

$$i\partial_t B_{\mu e} \simeq - \frac{e^{i \omega_{\mu e} t}}{\omega_{\mu e}} b_{\mu e} n_{\mu e}^2 V_{\mu e} \times \int \int \int r d\rho d\zeta \Phi_{\mu e} \int d\theta G_{e}^{c(2M_e - M_o)} \theta \times \sum_{\mu_1 \mu_2} (\omega_{\mu2o} + \omega_{\mu1o})^2 b_{\mu1o} b_{\mu2o} \Phi_{\mu_1o} \Phi_{\mu2o} \times B_{\mu_1o} + B_{\mu_2o} e^{i(\omega_{\mu2o} + \omega_{\mu1o})t}.$$ (5.3b)

Using Eq. (4.1) and after integrating in $\theta$, the only non-zero terms left in the right-hand sides of Eqs. (5.3a) are the ones satisfying an extended set of momentum matching conditions:

- difference frequency generation, ($e o \rightarrow o$):
  $$\mu_2 - (\mu_1 - g) + m = \mu, \quad (5.4a)$$

- sum frequency generation, ($o o \rightarrow e$):
  $$\mu_2 + (\mu_1 - g) + m = \mu, \quad (5.4b)$$

and describing all accounted for three wave mixing processes. Each of these frequency sum and frequency difference processes has its own frequency mismatch parameter,

- difference frequency generation:
  $$\varepsilon_{\mu2o1o,m} = \omega_{\mu2e} - \omega_{\mu1o} - \omega_{\mu o}, \quad (5.5a)$$

- sum frequency generation:
  $$\varepsilon_{\mu2o1o,m} = \omega_{\mu2o} + \omega_{\mu1o} - \omega_{\mu e}. \quad (5.5b)$$

Here and below an index in the top row of indices indicates polarization of a photon with the respective momentum index positioned in the bottom row. Thus, $\varepsilon_{\mu2o1o,m}$ are the the rank-4 frequency mismatch tensors in $\mu$ and $m$. Frequency and momentum matching considerations in Section 4, see Eqs. (4.12), (4.13), map onto the frequency mismatch tensors as $\varepsilon_{\mu2o1o,m} = - \varepsilon_{\mu o1o,m}$. After integrals are taken, Eqs. (5.3) become a system of the ordinary differential equations for $B_{\mu_{oe}}$.

$$i\partial_t B_{\mu o} = - \sum_{\mu_1 \mu_2 m} \gamma_{\mu2o1o,m} \hat{\gamma}_{\mu_2o + \mu_1 - g - m} \times G_{e} B_{\mu_1o} B_{\mu_2e} \exp \{-i \varepsilon_{\mu2o1o,m} \}, \quad (5.6a)$$

$$i\partial_t B_{\mu e} = - \sum_{\mu_1 \mu_2 m} \gamma_{\mu2o1o,m} \hat{\gamma}_{\mu_2o - \mu_1 - g - m} \times G_{e} B_{\mu_1o} B_{\mu_2e} \exp \{-i \varepsilon_{\mu2o1o,m} \}. \quad (5.6b)$$

Here the Kronecker symbol $\delta_{\mu_2o,\mu_1} = 1$ for $\mu_1 = \mu_2$, and is zero otherwise. Combinations of indices in $\hat{\gamma}$’s inside Eqs. (5.6) express the momentum matching conditions in Eqs. (5.4). Nonlinear coefficients $\gamma_{\mu2o1o,m}$ are the rank-4 tensors with the same index arrangements as in the frequency mismatch tensors,

$$\gamma_{\mu2o1o,m} = \frac{2(\omega_{\mu2e} - \omega_{\mu1o})^2 b_{\mu2e} b_{\mu1o}}{\omega_{\mu o} b_{\mu o}^2} \times \frac{2\pi}{\mu o} \int \int \int r d\rho d\zeta \Phi_{\mu e} \Phi_{\mu o} \Phi_{\mu e}, \quad (5.7a)$$

$$\gamma_{\mu2o1o,m} = \frac{(\omega_{\mu2o} + \omega_{\mu1o})^2 b_{\mu1o} b_{\mu2o}}{\omega_{\mu e} b_{\mu e}^2} \times \frac{2\pi}{\mu e} \int \int \int r d\rho d\zeta \Phi_{\mu o} \Phi_{\mu 2o} \Phi_{\mu e}. \quad (5.7b)$$

To fully set parameters for Eqs. (5.6), one has to specify elements of $\varepsilon_{\mu2o1o,m}$ and $\gamma_{\mu2o1o,m}$. Momentum matching conditions (5.4) fix, e.g., $\mu_2$, thereby reducing the number of nonzero tensor elements. For every quasi-phase matching order, $m$, one still needs to fix $\sim N^2$ constants. Doing so is not a problem for the frequency offset tensors, but knowing only $\gamma_{\mu2o1o,m}$ takes calculating a two dimensional integral. This task becomes impractical already for $N \sim 10^2$. However, if the research with $\chi^{(2)}$ microresonators is to progress to the generation of the octave and wider combs, and to designing of emission of resonance radiation, see, e.g., [29, 74, 75], then dispersion of nonlinear interaction is desirable to account for.

One approach to account for changes in values of $\gamma_{\mu2o1o,m}$ follows from the consideration, that initiation of spectral broadening happens through those $B_{\mu_1o} B_{\mu_2o}$ products, where one, or both, of the participating photons is the pump one. Thus, fixing $\mu_1 = 0$ and using momentum matching to find $\mu_2$ give $\mu_2 = - m - g$ for the frequency difference terms and $\mu_2 = - m + g$ for the sum-frequency ones. $m = \pm g$ is also a natural choice. Hence, using a substitution

$$\gamma_{\mu2o1o,m} \rightarrow \gamma_{\mu2o1o,m} \rightarrow \gamma_{\mu2o1o,m} \gamma_{\mu o}, \quad (5.8a)$$

$$\gamma_{\mu2o1o,m} \rightarrow \gamma_{\mu2o1o,m} \gamma_{\mu o}, \quad (5.8b)$$

allows to retain main features of the dispersion of $\gamma_{\mu2o1o,m}$ coefficients.
Eqs. (5.6) now become
\begin{align}
 i \partial_t B_{\mu o} &= -\gamma_{\mu o} \sum_{\mu_1 \mu_2 m} \delta_{\mu_2,\mu+m_1-g-m} G_m B_{\mu_1 o} B_{\mu_2 e} \\
 &\quad \times \exp\{-it\varepsilon_{\mu_2,\mu_1,\mu,m}\}, \quad (5.9a) \\
 i \partial_t B_{\mu e} &= -\gamma_{\mu e} \sum_{\mu_1 \mu_2 m} \delta_{\mu_2,\mu+m_1+g-m} G_m B_{\mu_1 o} B_{\mu_2 o} \\
 &\quad \times \exp\{-it\varepsilon_{\mu_2,\mu_1,\mu,m}\}. \quad (5.9b)
\end{align}

Here, the number of nonlinear coefficients to be set is 2N and the number of the respective double integrals to be taken is N.

Let us introduce more approximations for the sake of elaborating more explicit forms for γμ. We first use Eq. (5.10) and approximate ωμe − ω0o = ω0o + D1oμ + \(O(D2sμ^2)\), \(ωμ2 + ω0o = 2ω0o + D1oμ + \(O(D2sμ^2)\)). Thus,
\begin{align}
\gamma_{\mu o} &\simeq 2ω0o \left(1 + \frac{2D1oμ}{ω0o}\right) \\
&\times \frac{b_{μo}b_{o}^2}{b_{μo}b_{o}^2} \frac{2π}{ω0o} \int r dr dz d31 \Phi_{μo} \Phi_{o} \Phi_{μo}, \quad (5.10a) \\
\gamma_{μe} &\simeq 2ω0o \left(1 + \frac{D1oμ}{ω0o}\right) \\
&\times \frac{b_{μo}b_{o}^2}{b_{μo}b_{o}^2} \frac{2π}{ω0o} \int r dr dz d31 \Phi_{μo} \Phi_{o} \Phi_{μe}. \quad (5.10b)
\end{align}

Eqs. (5.10) account for dispersion of nonlinear coefficients that originates in the frequency pre-factors, see round brackets, and for dispersion of the mode profiles within the modal group around the pump and second harmonic fields, see expressions after ‘×’. Pump (ordinary) and second harmonic (extraordinary) are separated by an octave, therefore the mode profile change between them can be significant. However, the mode profile changes within the ordinary and extraordinary spectra can be disregarded to facilitate further transparency of the coefficient structure,
\begin{equation}
\gamma_{μ o} \simeq γ_{0 o} \left(1 + \frac{2D1oμ}{ω0o}\right), \quad γ_{μ e} \simeq γ_{0 e} \left(1 + \frac{D1oμ}{ω0o}\right). \quad (5.11)
\end{equation}

Eqs. (5.11) represent a reasonable approximation, that captures the linear in μ change of nonlinear interaction strength. In the real space this dependence is associated with the self-steepening effects, see Section 8A. It becomes more important for shorter resonators with higher repetition rates. If \(D1s/2π \sim 0.1\)THz then μ ~ 100 makes \(D1s/ω0o \sim 0.1\), which complies with approximations of Eqs. (5.11) and, at the same time, makes dispersion of nonlinearity appreciable. Taking \(D1s/2π \sim 1\)THz suggests using Eqs. (5.5), (5.7).

To get \(γ_{0 s}\) in Eqs. (5.11) one should use Eqs. (5.10). Integrals there can be roughly approximated using Gaussian mode profiles and \(r dr \approx r_0 dx; \quad 2π \int Φ_{0 o}^2 Φ_{e} rdrdz/V₀o \approx \frac{4}{3}\). Hence, \(γ_{0 o}\) are estimated as
\begin{equation}
γ_{0 o} \approx \frac{4d_{31}ω0o b_{o}e}{3n_{0 o}^2}, \quad γ_{0 e} \approx \frac{4d_{31}ω0o b_{o}e}{3n_{0 e}^2 b_{o}e}. \quad (5.12)
\end{equation}

Recalling Eq. (2.7) and taking \(n_{0 o} = 2.2, S_{0 o} = 50μm^2, S_{0 e} = 30μm^2\) we find \(b_{o o} \approx 1.3 \cdot 10^6, b_{o e} \approx 1.7 \cdot 10^6 W^{-1/2}/V/m\). Then, \(d_{31} = 4.8pm/V\) and \(ω0o/2π = 200THZ\) give \(γ_{0 o}/2π \approx 350, γ_{0 e}/2π \approx 270 MHz/W^{1/2}\).

VI. PUMP AND LOSS

We assume that a microresonator is pumped into a single ordinarily polarised mode, μ = 0, and that the laser frequency \(ω_p\) is tuned close to \(ω_{0 o}\). If \(H^2\) is the intracavity pump power that builds in the μ = 0 mode in the quasi-linear regime of operation and at the exact resonance, \(ω_{0 o} = ω_p\), then the pump and the finite linewidth effects can be incorporated to the model via a phenomenological substitution
\begin{align}
\hat{H}^2 &= \frac{η}{π} F W, \quad (6.2)
\end{align}
where η is the coupling efficiency into a resonator mode, η = \(k_c/κ_{0 o} < 1\), where \(k_c\) is the coupling pump rate, \(F = D_{1 o}/κ_{0 o}\) is the cavity finesse, or the power enhancement factor, which is typically 10³ and above for high-quality factor microresonators. Theory of power enhancement effects in ring cavities can be found in, e.g., Ref. [73].

Thus, the coupled-mode equations ready to be used for numerical modelling of practical experimental setups are
\begin{align}
\hat{H}B_{μ o} &= -i\frac{4}{3}κ_{μ o} B_{μ o} - \hat{δ}_{μ o} \hat{H}e^{i(ω_{μ o} - ω_p)t} \\
&\quad - γ_{μ o} \sum_{μ_1 μ_2 m} \hat{δ}_{μ_2, μ_1 + μ - m} G_m B_{μ_1 o}^* B_{μ_2 e} e^{-i(ω_{μ_2} - ω_{μ_1} - ω_p)t}, \quad (6.3a) \\
\hat{H}B_{μ e} &= -i\frac{4}{3}κ_{μ e} B_{μ e} \\
&\quad - γ_{μ e} \sum_{μ_1 μ_2 m} \hat{δ}_{μ_2, μ_1 + μ - m} G_m B_{μ_1 o}^* B_{μ_2 o} e^{-i(ω_{μ_2} + ω_{μ_1} - ω_p)t}. \quad (6.3b)
\end{align}

Quality factors between 10⁶ and 10⁷ would correspond to \(κ_{μ s}/2π\) varying in a range from below one to tens of MHz, with the tendency towards smaller quality factors for higher frequencies.

VII. PSEUDO-SPECTRAL FORM OF COUPLED-MODE EQUATIONS

Eqs. (6.3) are now ready to be set as an initial value problem and integrated in time with a suitable solver, including the variable step ones. However, nonlinear sums
remain a bottleneck in the multi-mode regime, since one should be summing up $\sim N$ exponential terms in $2N$ equations. Here we address how this can be handled efficiently using Fourier transform, that gives $N \ln N$ scaling. Expressing and computing multi-mode Kerr nonlinearity (four-wave mixing) via Fourier transforms has been discussed in Refs. [61, 70]. This is a so-called pseudo-spectral approach. It originates in solving quantum mechanical Schrödinger equation with a trapping potential using a basis of the free space eigenstates [63].

To achieve pseudo-spectral formulation, we first introduce detunings $\delta_{\mu\nu}$ between the laser frequency, $\omega_p$, and frequencies of the ordinary resonator modes, and $\delta_{\mu\nu}$ between 2$\omega_p$ and the extraordinary ones,

$$\delta_{\mu\nu} = \omega_{\mu\nu} - \omega_p, \quad (7.1a)$$
$$\delta_{\mu\nu} = \omega_{\mu\nu} - 2\omega_p. \quad (7.1b)$$

We also define new mode amplitudes, $Q_{\mu\nu}$,

$$Q_{\mu\nu} = B_{\mu\nu} e^{-i\delta_{\mu\nu} t}, \quad (7.2)$$

and the envelope functions $Q_s$,

$$Q_s = \sum_\mu Q_{\mu s} e^{i\mu \theta}, \quad s = o, e. \quad (7.3)$$

New amplitudes and the envelopes are linked as

$$Q_{\mu s} = \int_0^{2\pi} Q_s e^{-i\mu \theta} \frac{d\theta}{2\pi}. \quad (7.4)$$

Let us note here, that frequency mismatch tensors, Eqs. (7.3), are straightforwardly re-expressed via detunings:

$$\varepsilon_{\mu_2\mu_1\mu m}^{oo} = \delta_{\mu_2 e} - \delta_{\mu_1 o} - \delta_{\mu m o}, \quad (7.5a)$$
$$\varepsilon_{\mu_2\mu_1\mu m}^{oe} = \delta_{\mu_2 o} + \delta_{\mu_1 o} - \delta_{\mu m e}. \quad (7.5b)$$

Replacing $B_{\mu\nu}$ with $Q_{\mu\nu}$ in the nonlinear parts of Eqs. (4.3) we obtain

$$i\partial_t B_{\mu\nu} = -i\frac{1}{2} \kappa_{\mu\nu} \left( B_{\mu\nu} - \hat{\delta}_{\mu, o} \mathcal{H} e^{i\delta_{\mu\nu} t} \right) - \gamma_{\mu\nu} e^{i\delta_{\mu\nu} t} \sum_{\mu_1\mu_2 m}^{\mu_1\mu_2 m} \hat{\delta}_{\mu_2, \mu + \mu_1 - g - m} G_m Q_{\mu_1 o} Q_{\mu_2 e}, \quad (7.6a)$$
$$i\partial_t B_{\mu e} = -i\frac{1}{2} \kappa_{\mu e} B_{\mu e} - \gamma_{\mu e} e^{i\delta_{\mu e} t} \sum_{\mu_1\mu_2 m}^{\mu_1\mu_2 m} \hat{\delta}_{\mu_2, \mu - \mu_1 + g - m} G_m Q_{\mu_1 o} Q_{\mu_2 e}. \quad (7.6b)$$

Recalling momentum matching conditions, Eqs. (7.3), we use integral representations of the Kronecker $\delta's$, i.e.,

$$\int \frac{d\theta}{2\pi} e^{i(p_{\mu_2 \mu_1} + g_{\mu_2} - m - \mu_1) \theta} = \frac{1}{2\pi} \int \frac{d\theta}{2\pi} e^{i(p_{\mu_2 \mu_1} + g_{\mu_2} - m - \mu_1) \theta} = \frac{1}{2\pi} \int \frac{d\theta}{2\pi} e^{i(p_{\mu_2 \mu_1} + g_{\mu_2} - m - \mu_1) \theta},$$

in the sum terms in Eqs. (7.6). Applying Eqs. (7.4), (7.11) gives

$$i\partial_t B_{\mu o} = -i\frac{1}{2} \kappa_{\mu o} \left( B_{\mu o} - \hat{\delta}_{\mu, o} \mathcal{H} e^{i\delta_{\mu o} t} \right) - \gamma_{\mu o} e^{i\delta_{\mu o} t} \int_0^{2\pi} (G e^{i\theta} Q_o^* Q_e) e^{-i\theta} \frac{d\theta}{2\pi}, \quad (7.7a)$$
$$i\partial_t B_{\mu e} = -i\frac{1}{2} \kappa_{\mu e} B_{\mu e} - \gamma_{\mu e} e^{i\delta_{\mu e} t} \int_0^{2\pi} (G e^{-i\theta} Q_o^2) e^{-i\theta} \frac{d\theta}{2\pi}. \quad (7.7b)$$

Eqs. (7.7) is the central result of this work. They replace computationally demanding nonlinear sums of the multiple products of the mode amplitudes with Fourier transforms of products of the envelope functions. The latter is readily expressed via Fourier transforms of the amplitudes themselves, see Eqs. (7.5). Importantly, the real space quasi-phase-matching grating profiles are incorporated seamlessly and approximation free into this approach, and effectively play the role of an axillary field amplitude. One could also choose to account only for the leading order phase matching provided by the grating, which is accomplished via a substitution $G(\theta)e^{i\theta} \rightarrow G_{x,y}$, see Eq. (7.11).

**VIII. ENVELOPE EQUATIONS**

It is more handy for analytical work, but, at the same time, could be computationally more demanding to move to the $Q$-only formulation by replacing $B_{\mu\nu}$ with $Q_{\mu\nu}$ in the linear terms of Eqs. (7.3),

$$i\partial_t Q_{\mu o} = \delta_{\mu o} Q_{\mu o} - i\frac{1}{2} \kappa_{\mu o} \left( Q_{\mu o} - \hat{\delta}_{\mu, o} \mathcal{H} \right) - \gamma_{\mu o} \int_0^{2\pi} (G e^{i\theta} Q_o^* Q_e) e^{-i\theta} \frac{d\theta}{2\pi}, \quad (8.1a)$$
$$i\partial_t Q_{\mu e} = \delta_{\mu e} Q_{\mu e} - i\frac{1}{2} \kappa_{\mu e} Q_{\mu e} - \gamma_{\mu e} \int_0^{2\pi} (G e^{-i\theta} Q_o^2) e^{-i\theta} \frac{d\theta}{2\pi}. \quad (8.1b)$$

Retaining the grating profile $G(\theta)$ in Eqs. (8.1) prevents taking the full advantage of working in the reference frame rotating with the $D_{1D}$ rate. Replacing an integral in Eqs. (8.1) with an equivalent $\sum_{\mu_1 \mu_2 m}$, one finds that the nonlinear terms are evolving with frequencies given, in the leading order, by $||\delta_{\mu_1 o} - \delta_{\mu_1 o}||e|\sim D_{1e} \mu$ and $||\delta_{\mu_1 o} + \delta_{\mu_1 o}||\sim D_{1o} \mu$. At the same time, oscillation rates of the nonlinear terms in Eqs. (7.7) are given by $\varepsilon_{\mu_2\mu_1\mu m}^{oe}$, see Eqs. (7.5). One can readily show that in the leading order those are $D_{1o} / 2\pi \simeq 21GHz$ and $D_{1e} / 2\pi \simeq 19GHz$ in a millimetre scale LiNbO$_3$ microresonator Ref. [38]. This would give an order of magnitude difference in the time steps needed to achieve the same numerical accuracy if the two systems are solved with the same method and all parameters taken equal.

To derive the envelope, Lugato-Lefevel like, equations, we take Eqs. (5.1), neglect by the linewidth dispersion,
i.e., $\kappa_{\mu\nu} = \kappa_{\nu\mu}$, and account for dispersion of nonlinearity using an approximate Eq. (5.11). Transforming back to the physical space one obtains a system of the envelope equations with self-steepening terms,

$$i\partial_t Q_o = D_{10} Q_o + (-i D_{11} \partial_\theta - i \frac{1}{\tau_2} D_{20} \partial_\theta^2 + i \frac{1}{\tau_3} D_{30} \partial_\theta^3 + \ldots) Q_o$$

$$-\frac{i}{2} \kappa_{\mu\nu} \left(Q_o - H\right)$$

$$-\gamma_0 e \left(1 - i \frac{2 D_{11}}{\omega_{00}} \partial_\theta\right) G e^{i g \theta} Q_o^* Q_e, \quad (8.2a)$$

$$i\partial_t Q_e = D_{00} Q_e + (-i D_{01} \partial_\theta - \frac{1}{\tau_2} D_{21} \partial_\theta^2 + \frac{1}{\tau_3} D_{31} \partial_\theta^3 + \ldots) Q_e$$

$$-\frac{i}{2} \kappa_{\mu\nu} Q_e$$

$$-\gamma_0 e \left(1 - i \frac{D_{11}}{\omega_{00}} \partial_\theta\right) G e^{-i g \theta} Q_o^2. \quad (8.2b)$$

These equations, but without self-steepening, 3rd order dispersion and quasi-phase-matching terms, have been previously used by us in Refs. [38, 66, 67]. Physical values of the self-steepening coefficients are discussed at the end of Section 5 above.

**IX. NONLINEAR SHIFT OF THE PUMP RESONANCE: CHI-2 VS CHI-3**

Here we present a brief evaluation and comparison of the $\chi^{(2)}$ and Kerr induced resonance shifts in microresonators. An important observation in this regard is that detuning $\delta_{0e}$ is controlled on one side by the pump frequency, and on the other by phase matching and/or resonator dispersion. Indeed,

$$\delta_{0e} = 2 \delta_{0o} - \varepsilon, \quad (9.1)$$

where $\varepsilon$ is the cavity resonance frequency mismatch parameter defined in Eq. (9.2). We assume that phase-matching has been arranged to give $|\varepsilon|$ that is sufficiently large to dominate pump detuning and linewidth and sufficiently small to give a non-negligible second harmonic, i.e., $D_{1N} > |\varepsilon| \gg \kappa_{0s}$. Then, assuming the single mode operation,

$$Q_{0e} \simeq -\frac{\gamma_{0e}}{\varepsilon} G_s Q_o^2. \quad (9.2)$$

Substituting Eq. (9.2) into Eq. (8.13), one finds that $\chi^{(2)}$ nonlinearity induces an effective, or cascaded $\chi^{(3)}$, Kerr effect for the ordinary wave, which gives the following nonlinear shift of $\omega_{0o}$ ($g_{2g} = 1$):

$$\Delta_{cas} = \frac{\gamma_{0o} \gamma_{0e}}{\varepsilon} |Q_{0o}|^2 \sim \frac{\omega_{0o}}{2 S_{0o} n_{0o}} \frac{16 Z_{vac} \omega_{0o} d_{31}^2}{9 n_{0o}^2 \varepsilon} |Q_{0o}|^2. \quad (9.3)$$

Using Ref. [61], the shift of $\omega_{0o}$ due to intrinsic Kerr effect is

$$\Delta = -\frac{\omega_{0o}}{2 S_{0o} n_{0o}} n_2 |Q_{0o}|^2. \quad (9.4)$$

We take the intrinsic Kerr coefficient for LN as $n_2 \simeq 5 \cdot 10^{-19} \text{m}^2/\text{W}$, noting that there is some spread of values met in the literature.

Comparing Eqs. (9.3) and (9.4), leads to the cascaded, $\chi^{(2)}$ induced, Kerr coefficient

$$n_{2cas} = -\frac{16 Z_{vac} \omega_{0o} d_{31}^2}{9 n_{0o}^2 \varepsilon}. \quad (9.5)$$

Choosing, as an example, $\varepsilon/2\pi = 1 \text{GHz}$ gives $n_{2cas} \simeq 6 \cdot 10^{-16} \text{m}^2/\text{W}$, which is three orders of magnitude above the intrinsic $n_2$. For smaller $\varepsilon$, i.e., better phase matching, dominance of $n_{2cas}^2$ will increase according to $n_{2cas}^2 \sim 1/\varepsilon$. For $|\varepsilon| < \kappa_{0e}$, this scaling should be generalised to include saturation of $n_{2cas}^2$ with power and detuning effects [66]. Threshold for the comb generation via intrinsic Kerr nonlinearity in integrated LN resonators is $\lesssim 100 \text{mW}$ and scales inversely with $n_2$ [33]. If the cascaded nonlinearity is triggered, then according to $n_{2cas}/n_2 \sim 10^3$, the threshold is expected to decrease to $100 \mu\text{W}$ and less. Exploring weighting of $\chi^{(2)}$ vs $\chi^{(3)}$ effects further can easily constitute a separate investigation and we refer a reader to Refs. [34, 40, 66, 80] for more information. Impacts of Raman and slow photorefractive responses of LN on comb generation have been analysed in, e.g., [63, 60].

**X. SUMMARY**

We have presented an ab-initio derivation of the coupled-mode equations describing nonlinear wave mixing processes in microresonators with quadratic nonlinearity and quasi-phase-matching. Main features of our coupled-mode formulation given by Eqs. (1.1) are - (i) nonlinear terms are evaluated pseudo-spectrally, i.e., using Fourier transforms of the products of the real space envelope functions; (ii) number of nonlinear coefficients to be calculated to account for dispersion of the nonlinear interaction is optimized, Eqs. (2); (iii) arbitrary profiles of the quasi-phase-matching gratings naturally enter the pseudo-spectral formulation.

While we considered in details an example of phase matching between ordinary and extraordinary waves in an LN crystal mediated by the $d_{31}$ coefficient, we also provide a full tensor formulation of the nonlinear response, that includes all other types of three-wave mixing, see Eqs. (8.7), and allows extensions of our approach. We further demonstrate that the coupled-mode Eqs. (7.7) with the nonlinear coefficients approximated by Eqs. (5.11) are formally equivalent to a pair of the envelope equations, Eqs. (8.2), with self-steepening terms. Balance of the time-scales involved suggests that Eqs. (7.7) are computationally advantageous over Eqs. (8.2). Opportunities for future studies concerning both physics and numerics related aspects of the problem and also the mapping of the models onto a rich variety of experimental settings are numerous.
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