Spatiotemporal Model for Kerr Comb Generation in Whispering Gallery Mode Resonators

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We establish an exact partial differential equation to model Kerr comb generation in whispering-gallery mode resonators. This equation is a variant of the Lugiato-Lefever equation that includes higher-order dispersion and nonlinearity. This spatio-temporal model, whose main variable is the total intracavity field, is significantly more suitable than the modal expansion approach for the theoretical understanding and the numerical simulation of wide-span combs. It allows us to explore pulse formation in which a large number of modes interact cooperatively. This versatile approach can be straightforwardly extended to include higher-order dispersion, as well as other phenomena like Raman, Brillouin and Rayleigh scattering. We demonstrate for the first time that when the dispersion is anomalous, Kerr comb generation can arise as the spectral signature of dissipative cavity solitons, leading to wide-span combs with low pumping.

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The development of frequency combs – equidistant frequency lines from a short-pulse laser – revolutionized the measurement of frequencies [1] and has opened up a host of potential applications in fundamental and applied physics, including the measurement of physical constants, the detection of earth-like planets, chemical sensing, the generation, measurement, and distribution of highly accurate time, and the generation of low-phase-noise microwave radiation [2]. Ti:sapphire lasers were used as the original source of frequency combs, but in the past seven years, alternative fiber laser sources have developed [2]. Recently, Del’Haye, et al. [3] demonstrated that it is possible to use the whispering gallery modes in microresonators in combination with the Kerr effect to generate an equidistant frequency comb that is also referred to as a Kerr comb. Since many applications in both fundamental and applied science would benefit from the small size, simplicity, robustness, and low power consumption of these whispering gallery mode sources, a considerable worldwide effort has gone into understanding and controlling them [4]. In particular, there have been several efforts to develop mathematical models of these sources [5-8], but all the efforts to date have serious drawbacks.

A complete modal expansion has been derived to describe the growth of the Kerr combs from noise [5, 6]. This model predicts a cascaded growth in which a primary comb is first generated, which then generates a secondary comb, and later higher order combs. This model is in complete agreement with experiments [5]. However, it is difficult and computationally expensive to use this mode expansion beyond the primary comb generation because the number of modes that must be kept in a calculation grows like the third power of time. Moreover, it is difficult to study pulse formation in this model, since a large number of modes interact cooperatively. Pulse formation plays a critical role in comb generation. It is desirable to find a spatio-temporal model that would be analogous to the Haus modelocking equation (a variant of the nonlinear Schrödinger equation) that has been used with great success to study modelocked lasers [9]. However, this equation is not itself appropriate for whispering gallery mode resonators. This equation assumes that pulses are isolated, and it does not take into account the periodic boundary conditions and the fundamental role that continuous wave pumping and dissipation play in the evolution [8].

In this letter, we show that the Lugiato-Lefever equation (LLE) [10] is the appropriate spatio-temporal model of whispering gallery mode resonators. We demonstrate that the previously-derived modal expansion is equivalent to a variant of the LLE that includes higher-order dispersion and nonlinearity, and the standard LLE closely approximates the modal expansion. We then use this model to study pulse formation and determine conditions under which multiple pulses (rolls) and single pulses (dissipative solitons) form in the cavity. We show that a broadband comb is obtained when a single dissipative soliton forms.

The LLE can be considered a variant of the nonlinear Schrödinger equation (NLSE) that includes damping, driving, and detuning. It has been the subject of intensive mathematical study [11-13], and it has been experimentally demonstrated that this model can be applied to

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fiber ring resonators \[14\]. Unexpected phenomena such has convective instability \[15\] and excitability \[16\] are also known occur in this system. The identification of the LLE as the fundamental equation governing the field evolution in whispering gallery mode resonators allows us to take advantage of this prior work, while at the same time suggesting efficient computational methods for studying the field evolution, including Kerr comb generation.

Our starting point is the modal equations that were derived in ref. \[6\]. The modal structure of the whispering gallery mode resonators is well-understood. It has been shown that these resonators can sustain several families of eigenmodes that trap light inside the cavity by total internal reflection. We are only interested in the fundamental family of modes that can be characterized by their toroidal structure. Provided that the polarization is fixed, the members of this family are unambiguously defined by an integer wavenumber \( ℓ \) that characterizes each member’s angular momentum and can be interpreted as the total number of reflections that a photon makes during one round trip in the cavity.

We denote the eigenmode of the pumped mode as \( ℓ_0 \). If we restrict ourselves to the spectral neighborhood of \( ℓ_0 \), the eigenfrequencies can be expanded in a Taylor series, whose first three elements are

\[
ω_ℓ = ω_ℓ₀ + ζ₁(ℓ − ℓ₀) + \frac{1}{2}ζ₂(ℓ − ℓ₀)², \tag{1}
\]

where \( ω_ℓ₀ \equiv ω₀ \) is the eigenfrequency at \( ℓ = ℓ₀ \), \( ζ₁ = dω/dℓ |_{ℓ=ℓ₀} = Δω_{FSR} \) is the free-spectral range of the resonator or the intermodal angular frequency, and \( ζ₂ = d²ω/dℓ² |_{ℓ=ℓ₀} \) is the second-order dispersion coefficient. The quantity \( ζ₂ \) corresponds to \( ζ \) in refs. \[5\] \[6\]. In the case of a disk resonator with main radius \( a \), we find \( ζ₁ = c/n₀a \), where \( c \) is the velocity of light and \( n₀ \) is the index of refraction at \( ω₀ \). This intermodal angular frequency is linked to the round-trip period of a photon through the resonator as \( T = 2π/ζ₁ \). The second-order dispersion \( ζ₂ \) denotes the lowest-order deviation from frequency equistance of the modes. When \( ζ₂ = 0 \), the eigenfrequencies are equidistant to lowest order and are separated by \( ζ₁ \). The dispersion is normal when \( ζ₂ < 0 \) and anomalous when \( ζ₂ > 0 \). In fact, \( ζ₂ \) is the sum of two contributions – the geometrical dispersion (generally normal) and the material dispersion (which can be normal or anomalous). Explicit expressions are given in refs. \[5\] \[6\] for a spherical resonator.

We now consider the elements of the modal expansion in a range of \( ℓ \)-values in which the expansion of Eq. \[1\] is valid. The slowly varying envelopes \( A_ℓ \) obey the equations \[5\] \[6\]

\[
\frac{dA_ℓ}{dt} = -\frac{1}{2}Δω_ℓ A_ℓ + \frac{1}{2}Δω_ℓ F_ℓ e^{i(Ω₀ − ω_ℓ) t} δ(ℓ − ℓ₀) \tag{2}
\]

\[
−ig₀ \sum_{ℓ_m,ℓ_n,ℓ_p} A_{ℓ_m} A_{ℓ_n}^{∗} A_{ℓ_p} e^{i[ω_{ℓ_m} − ω_{ℓ_n} + ω_{ℓ_p} − ω_ℓ] t} \]

\[
x_{ℓ_m,ℓ_n,ℓ_p} δ(ℓ_m − ℓ_n + ℓ_p − ℓ), \]

where \( δ(x) \) is the Kronecker delta-function that equals 1 when \( x = 0 \) and equals zero otherwise.

The mode fields have been normalized so that \( |A_ℓ|^² \) corresponds to the photon number in the mode \( ℓ \). The mode bandwidth \( Δω_ℓ = ω_ℓ/Q_0 \) is inversely proportional to the loaded quality factor \( Q_0 \) and to the phonon lifetime \( τ_{qh} = 1/Δω_ℓ \). The four-wave mixing gain is \( g₀ = n₂cω₀^²/n₀^2V₀ \), where \( h \) is Planck’s constant, \( n₂ \) is the Kerr coefficient, and \( V₀ \) is the effective mode volume. The coefficient \( A_{ℓ_m,ℓ_n,ℓ_p}^{ℓ} \) indicates the mode overlap. The parameter \( F₀ \) denotes the amplitude of the external excitation, while \( Ω₀ \) is the angular frequency of the pump laser, and it is assumed to be close to \( ω₀ \). Typically, resonant pumping only occurs when \( |Ω₀ − ω₀| ∼ Δω₀ \).

The spatiotemporal slowly varying envelope of the total field \( A(θ, t) \) may now be written

\[
A(θ, t) = \sum_ℓ A_ℓ(t) e^{i(ω_ℓ − ω₀) t − i(ℓ − ℓ₀)θ}, \tag{3}
\]

where \( θ \in [-π, π] \) is the azimuthal angle along the circumference. From Eq. \[3\], it follows that

\[
\frac{∂A}{∂t} = \sum_ℓ \left[ \frac{dA_ℓ}{dt} + i(ω_ℓ − ω₀) A_ℓ \right] e^{i(ω_ℓ − ω₀) t − i(ℓ − ℓ₀)θ}. \tag{4}
\]

Equation \[3\] independently yields

\[
\frac{i²}{n} \frac{∂ⁿA}{∂θⁿ} = \sum_ℓ (ℓ − ℓ₀)ⁿ A_ℓ e^{i(ω_ℓ − ω₀) t − i(ℓ − ℓ₀)θ}, \tag{5}
\]

so that if we restrict ourselves in the degenerate case where \( A_{ℓ_m,ℓ_n,ℓ_p}^{ℓ} = 1 \) and \( Δω_ℓ = Δω₀ \), the evolution equation \[4\] can be rewritten as

\[
\frac{∂A}{∂t} = -\frac{1}{2}Δω₀ A - i|g₀| |A|^² A + \frac{1}{2}Δω₀ F₀ e^{iσt}
−ζ₁ A − \frac{ζ₂}{2} A \frac{∂²A}{∂θ²}, \tag{6}
\]

where \( σ = Ω₀ − ω₀ \) is the detuning between the laser and cavity resonance frequencies. It is useful to translate the frequency of the carrier envelope to remove the explicit time-dependence of the driving term by making the transformation \( A \to A \exp(ıσt) \). It is also useful to transform the \( θ \)-coordinate to remove the group velocity motion by making the transformation \( θ \to θ − ζ₁ t \mod[2π] \). When that is done, we find that Eq. \[6\] becomes

\[
\frac{∂A}{∂t} = -\frac{1}{2}Δω₀ A - iσ A + \frac{1}{2}Δω₀ F₀
−ig₀ |A|^² A − iζ₂ A \frac{∂²A}{∂θ²}. \tag{7}
\]

Finally, this equation can be rewritten in the form of the normalized Lugato-Lefever equation

\[
\frac{∂ψ}{∂τ} = -(1 + iα)ψ + |ψ|^²ψ - \frac{β}{2} \frac{∂²ψ}{∂θ²} + F, \tag{8}
\]
Hence, we would expect the stationary intra-cavity field \( \psi \) to be on the order of \( 1 \) in our theoretical analysis and numerical simulations. Note that in Eq. (8), the dimensionless time can be rewritten as \( \tau = \Delta \omega_0 t/2 \). The dimensionless parameters of this normalized equation are the frequency detuning \( \alpha = -2\sigma/\Delta \omega_0 \), the dispersion \( \beta = -2\zeta_2/\Delta \omega_0 \), and the external pump \( F = (2g_0/\Delta \omega_0)^{1/2} F_0 \). This LLE with periodic boundary conditions is the exact counterpart of the modal expansion as long as higher-order dispersion and the variation of \( \Delta \omega_0 \) and \( \Delta \omega_\ell \) can be neglected. Since the higher-order corrections can be calculated, it is always possible to check the validity of the LLE, and it will remain valid until the comb is nearly octave-spanning. As a consequence, all the conclusions that were previously obtained using the modal expansion and confirmed experimentally can also be obtained by solving the LLE. These two twin-models are however useful in different and complementary ways. On the one hand, the modal expansion must be used to determine threshold phenomena when a small number of modes are involved. On the other hand, the LLE is appropriate to use when many hundreds or thousands of modes interact since it does not refer to the individual modes. In particular, as we will show later, it is useful in the study of Kerr combs or pulse (soliton) growth and propagation in which a large number of modes interact cooperatively.

We now discuss the meaning and order of magnitude of the variables and parameters that appear in the dimensionless LLE. The detailed analysis of ref. [6] showed that the threshold value for the Kerr comb is given by \( |A|_{th}^2 = \Delta \omega_0/2g_0 \), which exactly corresponds to \( |\psi|_{th}^2 = 1 \). Hence, we would expect \( \psi \) to be on the order of \( 1 \) in our analytical and numerical simulations. Note that the stationary intra-cavity field \( \psi_0 \) before comb generation can be obtained by setting all the derivatives to zero in Eq. (8). The dimensionless time can be rewritten as \( t/2\tau_{ph} \), where we recall that \( \tau_{ph} \) is the photon lifetime, which is typically a few \( \mu s \) in ultra-high-Q whispering gallery mode resonators. Using the external field’s phase as our reference, the amplitude \( F \) is real and positive and \( F^2 \) is proportional to the external pump power. The real parameter \( \alpha \) equals the ratio of the detuning to half the linewidth, so that we expect to be off resonance when \( |\alpha| > 1 \). This parameter is easily tuned in experiments. The parameter \( \beta \) equals the ratio of the walkoff due to second-order dispersion to the half-linewidth. This parameter is negative for anomalous dispersion and positive for normal dispersion. It is a relatively small parameter. In refs. [5] [6] for example, it was found that \( \beta \sim -0.01 \) was sufficient to generate combs. In practice, the dispersion magnitude \( |\beta| \) should not be too large (~1), as it would mean that the deviation from equidistance of the mode frequencies would be too strong for the nonlinearity to compensate, and the emergence of a wide-span Kerr comb would be suppressed.

Numerical simulations were performed using the split-step Fourier algorithm, which is commonly used in simulations of the 1-D generalized NLSE. We note that this simulation method inherently assumes periodic boundary conditions because it is based on the fast Fourier transform (FFT). For studies of pulses in optical fibers – in which the pulse duration can often be many orders of magnitude smaller than the separation between pulses – this feature is often an annoyance that leads to boundary-induced artifacts. In our case, the physical boundary conditions are periodic. The split-step Fourier algorithm is therefore a remarkably cost-effective computational tool, enabling the simulation of Kerr comb dynamics with a laptop computer in a few minutes regardless of its spectral span, as opposed to a few days with the modal expansion for wide-span combs.

For the numerical simulation of the LLE, Eq. (8), we have considered a calcium fluoride resonator with a radius \( a = 2.5 \) mm. The polar eigenmode of the TE-polarized pump mode is \( \ell_0 = 14350 \), corresponding to a wavelength of 1560.5 nm and \( \omega_0 = 2\pi \times 192.24 \) THz in vacuum. The index of refraction is \( n_0 = 1.43 \). The res-
onator is critically coupled with a loaded quality factor $Q_0 = 3 \times 10^3$, corresponding to a central mode bandwidth of $\Delta \omega / r / Q \approx 2 \pi \times 64 \text{ kHz}$. The free spectral range is equal to $\Delta \omega_{\text{FSR}} = c_1 = 2 \pi \times 13.36 \text{ GHz}$.

In Fig. [1] we present simulation results that correspond to those that have already been obtained from the modal expansion, namely the multiple-FSR solution. It can be seen that the solution corresponds to the formation of “rolls” in the time domain. We take advantage of the LLE formulation to show particular solutions that would be difficult to observe in a strictly modal study. Figure [2] shows the formation of a single-peaked cavity soliton. This dissipative localized structure is a sub-critical Turing pattern. The figure corresponds to a single pulse of width $\Delta T \approx 500 \text{ fs}$, circulating inside the cavity with a round-trip time $T = 2 \pi / \Delta \omega_{\text{FSR}} \approx 75 \text{ ps}$. In the frequency domain, this pulse consists of several tens of mode-locked whispering gallery modes, whose frequencies have been nonlinearly shifted so that they are equidistant, as shown in Fig. [1]. Because this cavity soliton is subcritical, it emerges abruptly and at a low pump power. The solitonic Kerr combs do not grow as the pump power increases; instead, they are destroyed. By contrast, supercritical combs like the one shown in Fig. [1] have spectral components that grow in number and power as the external pump power grows. However, the dissipative cavity solitons are robust, and their full width at half maximum decreases with the dispersion parameter $|\beta|$.

For the simulation of wide-span combs, the LLE can be generalized to take into account higher-order dispersion ($\zeta_n = d^n \omega / d\xi^n |_{\xi = \xi_0} \neq 0$, with $n \geq 3$), non-degeneracy of the bandwidths ($\Delta \omega_\ell \neq \Delta \omega_0$), and spatial non-degeneracy of the eigenmodes ($\Lambda_{\ell m | \ell n | \ell p} \neq 1$). Indeed, these higher-order effects have to be taken into consideration for the simulation of octave-spanning combs. If we account for third-order dispersion and the first-order variation of $\Lambda_{\ell m | \ell n | \ell p}$, Eq. (6) becomes

\[
\frac{\partial A}{\partial \ell} = -\frac{1}{2} \Delta \omega_0 A - ig_0 |A|^2 A + \frac{1}{2} \Delta \omega_0 F e^{i \omega t} \left( -\zeta_1 \frac{\partial A}{\partial \theta} - i \frac{c_2}{2} \frac{\partial^2 A}{\partial \theta^2} + \frac{c_3}{6} \frac{\partial^3 A}{\partial \theta^3} + g_0 \left[ \eta_\ell \frac{\partial}{\partial \theta} (|A|^2 A) + 2 \eta_\kappa_\ell |A|^2 \frac{\partial A}{\partial \theta} - \eta_\kappa_\ell A^2 \frac{\partial A^*}{\partial \theta} \right] \right),
\]

where $\eta_\ell = \partial \Delta / \partial \ell$ for $\ell_m = \ell_n = \ell_p = \ell = \ell_0$, with $\eta_\kappa_\ell$, $\eta_\kappa_\ell$, and $\eta_\kappa_\ell$ being defined analogously. The details of the derivation are analogous to similar derivations of the NLSE with higher-order corrections [17]. When the bandwidth of the resonator field approaches the carrier frequency, the Taylor expansion in Eq. (1) is no longer valid, and one must use the full functional dependence of $\omega - \omega_\ell$ on $\ell$, by analogy to what is done in studies of supercontinuum generation.

In conclusion, we have demonstrated that the Kerr comb evolution in whispering gallery mode resonators can be modeled using the Lugiato-Lefever equation and its extensions. We have shown that low-threshold, wide-span combs can emerge as dissipative cavity solitons. With different parameters, rolls appear, corresponding to narrower-band combs. So, when the goal is to optimize the bandwidth a correct parameter choice is critical. Additionally, we demonstrated that the LLE can be extended to incorporate higher-order dispersion and nonlinearity, and we expect that it can be extended to include Rayleigh, Brillouin, and Raman scattering [18]. A key advantage of the spatiotemporal model that we have developed is that the LLE has already been the subject of extensive mathematical study, and it should be possible to take advantage of this earlier work to shed additional light on the dynamical properties of Kerr combs. We expect that a better understanding of Kerr comb generation in whispering gallery resonators will be the result, leading to new resonator designs that can produce octave-spanning combs.

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