Spatiotemporal Lugiato-Lefever formalism for Kerr-comb generation in whispering-gallery-mode resonators

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We demonstrate that frequency (Kerr) comb generation in whispering-gallery-mode resonators can be modeled by a variant of the Lugiato-Lefever equation that includes higher-order dispersion and nonlinearity. This spatiotemporal model allows us to explore pulse formation in which a large number of modes interact cooperatively. Pulse formation is shown to play a critical role in comb generation, and we find conditions under which single pulses (dissipative solitons) and multiple pulses (rolls) form. We show that a broadband comb is the spectral signature of a dissipative soliton, and we also show that these solitons can be obtained by using a weak anomalous dispersion and subcritical 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 earthlike 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], and there have been several efforts to develop mathematical models of these sources [5–7].

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 calculation time grows as the third power of the number of modes [6]. 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 spatiotemporal 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 [8]. Early research had investigated the modulational instability in a synchronously pumped nonlinear dispersive ring cavity, and predicted the formation of stable temporal dissipative structures for both the normal and the anomalous dispersion regime of the fiber [9,10]. In recent work, Matsko *et al.* [11] have used a two-time-scales approach similar to that of Haus [8], and they have built a spatiotemporal model that successfully predicted comb generation through modelocking and pulse formation.

In this article we show that a variant of the Lugiato-Lefever equation (LLE) [12] in which the evolution is in time and the conjugate (transverse) variable is the resonator's azimuthal angle is the appropriate spatiotemporal model for Kerr-comb generation in 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 when the bandwidth is small compared to the carrier frequency and does not approach an octave. We then use this model to study how multiple pulses (rolls) and single pulses (dissipative solitons) form in the cavity.

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 [13–15]. Unexpected phenomena such has convective instabilities [16] and excitability [17] are also known to 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

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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 wave number 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 eigennumber 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 N elements are

$$\omega_\ell = \omega_{\ell_0} + \sum_{n=1}^{N} \frac{\zeta_n}{n!}(\ell - \ell_0)^n, \qquad (1)$$

where ω_{ℓ_0} is the eigenfrequency at $\ell = \ell_0$, $\zeta_1 = d\omega/d\ell|_{\ell=\ell_0} = \Delta\omega_{\rm FSR}$ is the free-spectral range of the resonator or the intermodal angular frequency, and $\zeta_2 = d^2\omega/d\ell^2\big|_{\ell=\ell_0}$ is the second-order dispersion coefficient. In effect, we are making a polynomial fit of Nth order to the frequency ω_ℓ, which is a discrete function of ℓ. Since there are many thousands of frequencies and the ω_ℓ are smoothly varying, we may treat the ω_ℓ as a continuous function of ℓ and set the ζ_n equal to the Taylor expansion coefficients.

The quantity ζ_2 corresponds to ζ in Refs. [5,6]. In the case of a disk resonator with main radius a, we find $\zeta_1 = c/n_0 a$, where c is the velocity of light and n_0 is the index of refraction at ω_{ℓ_0}. This intermodal angular frequency is linked to the round-trip period of a photon through the resonator as $T = 2\pi/\zeta_1$. The second-order dispersion ζ_2 denotes the lowest-order deviation from frequency equistance of the modes. When $\zeta_2 = 0$, the eigenfrequencies are equidistant to lowest order and are separated by ζ_1. The dispersion is normal when $\zeta_2 < 0$ and anomalous when $\zeta_2 > 0$. In fact, ζ_2 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 $\mathcal{A}_\ell$ obey the equations [5,6]

$$\begin{aligned}\frac{d\mathcal{A}_\ell}{dt} &= -\frac{1}{2}\Delta\omega_\ell\,\mathcal{A}_\ell + \frac{1}{2}\Delta\omega_\ell\,\mathcal{F}_\ell\, e^{i(\Omega_0-\omega_\ell)t}\delta(\ell-\ell_0)\\ &\quad - i g_0 \sum_{\ell_m,\ell_n,\ell_p} \mathcal{A}_{\ell_m}\mathcal{A}^*_{\ell_n}\mathcal{A}_{\ell_p} e^{[i(\omega_{\ell_m}-\omega_{\ell_n}+\omega_{\ell_p}-\omega_\ell)t]}\\ &\quad \times \Lambda_\ell^{\ell_m\ell_n\ell_p}\delta(\ell_m-\ell_n+\ell_p-\ell), \end{aligned} \qquad (2)$$

where $\delta(x)$ is the Kronecker δ function that equals 1 when $x = 0$ and equals zero otherwise. The mode fields have been normalized so that $|\mathcal{A}_\ell|^2$ corresponds to the photon number in the mode ℓ. The mode bandwidth $\Delta\omega_\ell = \omega_\ell/Q_0$ is inversely proportional to the loaded quality factor Q_0 and to the photon lifetime $\tau_{{\rm ph},\ell} = 1/\Delta\omega_\ell$. The four-wave mixing gain is $g_0 = n_2 c\hbar\omega_{\ell_0}^2/n_0^2 V_0$, where $\hbar$ is Planck's constant, n_2 is the Kerr coefficient at $\ell = \ell_0$, and V_0 is the effective mode volume. The variation of the coefficient $\Lambda_\ell^{\ell_m\ell_n\ell_p}$ is due to variations in the mode overlap and the Kerr coefficient with mode number. The parameter $\mathcal{F}_0$ denotes the amplitude of the external excitation, while Ω_0 is the angular frequency of the pump laser, and it is assumed to be close to ω_{ℓ_0}. Typically, resonant pumping only occurs when $|\Omega_0 - \omega_{\ell_0}| \lesssim \Delta\omega_{\ell_0}$.

When the spectrum is restricted to the neighborhood of ℓ_0, then $\Lambda_\ell^{\ell_m\ell_n\ell_p} \simeq 1$, but when the spectrum begins to approach an octave of bandwidth, higher-order corrections, analogous to the higher-order terms in Eq. (1) must be kept.

At lowest order, we find

$$\begin{aligned}\Lambda_\ell^{\ell_m\ell_n\ell_p} &= 1 + \eta_\ell(\ell-\ell_0) + \eta_{\ell_m}(\ell_m-\ell_0)\\ &\quad + \eta_{\ell_n}(\ell_n-\ell_0) + \eta_{\ell_p}(\ell_p-\ell_0),\end{aligned} \qquad (3)$$

where $\eta_\ell = \partial\Lambda/\partial\ell$ is evaluated when ℓ, ℓ_m, ℓ_n, and ℓ_p are all equal to ℓ_0. The coefficients η_{ℓ_m}, η_{ℓ_n}, and η_{ℓ_p} are all analogously defined. From the symmetry of Eq. (2) under interchange of $\mathcal{A}_{\ell_m}$ and $\mathcal{A}_{\ell_p}$, it follows that $\eta_{\ell_m} = \eta_{\ell_p}$. As is the case for ω_ℓ, the quantity $\Lambda_\ell^{\ell_m\ell_n\ell_p}$ varies smoothly as a function of its arguments and may be treated as a continuous function, so that the coefficients in Eq. (3) correspond to the terms in a Taylor expansion. Since the mode overlap is a maximum when $\ell = \ell_m = \ell_n = \ell_p = \ell_0$, we expect that these first-order contributions will be dominated by variations of the Kerr coefficient due to changes in the mode volume and the contribution from the Raman effect. The second-order contributions from the decrease in the mode overlap will also become important as the bandwidth approaches an octave. A detailed investigation of the competing nonlinear contributions and their relative importance remains to be carried out [18].

The spatiotemporal slowly varying envelope of the total field $\mathcal{A}(\theta,t)$ may now be written

$$\mathcal{A}(\theta,t) = \sum_\ell \mathcal{A}_\ell(t)\exp[i(\omega_\ell - \omega_{\ell_0})t - i(\ell-\ell_0)\theta], \qquad (4)$$

where $\theta \in [-\pi,\pi]$ is the azimuthal angle along the circumference. From Eq. (4) it follows that

$$\frac{\partial\mathcal{A}}{\partial t} = \sum_\ell \left[\frac{d\mathcal{A}_\ell}{dt} + i(\omega_\ell - \omega_{\ell_0})\mathcal{A}_\ell\right] e^{[i(\omega_\ell-\omega_{\ell_0})t - i(\ell-\ell_0)\theta]}. \qquad (5)$$

Equation (4) independently yields

$$i^n\frac{\partial^n\mathcal{A}}{\partial\theta^n} = \sum_\ell (\ell-\ell_0)^n\mathcal{A}_\ell e^{[i(\omega_\ell-\omega_{\ell_0})t - i(\ell-\ell_0)\theta]}, \qquad (6)$$

so that if we set $\Delta\omega_\ell = \Delta\omega_{\ell_0}$, the evolution equation (5) can be rewritten as

$$\begin{aligned}\frac{\partial\mathcal{A}}{\partial t} &= -\frac{1}{2}\Delta\omega_{\ell_0}\mathcal{A} - i g_0|\mathcal{A}|^2\mathcal{A} + \frac{1}{2}\Delta\omega_{\ell_0}\mathcal{F}_0 e^{i\sigma t}\\ &\quad + \sum_{n=1}^{N} i^{n+1}\frac{\zeta_n}{n!}\frac{\partial^n\mathcal{A}}{\partial\theta^n}\\ &\quad + g_0\left[\eta_\ell\frac{\partial}{\partial\theta}(|\mathcal{A}|^2\mathcal{A}) + 2\eta_{\ell_m}|\mathcal{A}|^2\frac{\partial\mathcal{A}}{\partial\theta} - \eta_{\ell_n}\mathcal{A}^2\frac{\partial\mathcal{A}^*}{\partial\theta}\right],\end{aligned} \qquad (7)$$

where $\sigma = \Omega_0 - \omega_{\ell_0}$ is the detuning between the laser and cavity resonance frequencies. Note that while Eq. (7) could be used to account for a frequency dependent nonlinearity, it still neglects the frequency dependence of the absorption. 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 $\mathcal{A} \to \mathcal{A}\exp(i\sigma t)$. It is also useful

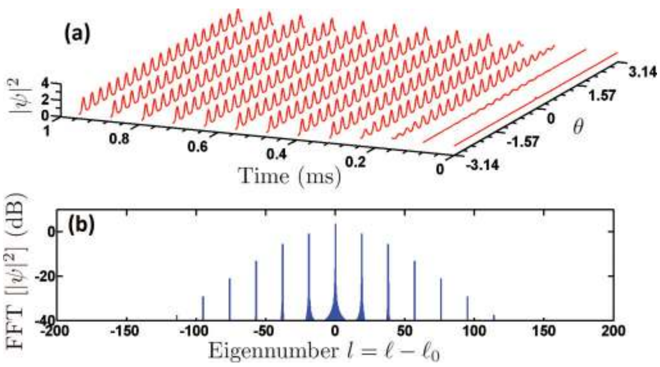

FIG. 1. (Color online) Multiple-FSR comb with $\alpha = 0$, $\beta = -0.0125$, and $F = 1.71$. The intracavity pump is $|\psi_0|^2 = 1.2$, so that it is above threshold $|\psi|^2_{\rm th} = 1$. The parameters correspond to Fig. 10(b) in Ref. [6]. (a) Time-domain dynamics that consists of 19 smooth pulses ("roll" Turing pattern solution). (b) FFT of the roll solution, corresponding to an order 19 multiple-FSR comb.

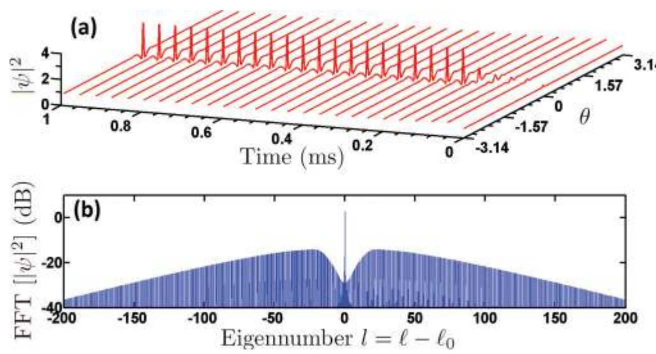

FIG. 2. (Color online) Temporal cavity soliton with $\alpha = 1.7$, $\beta = -0.002$, and $F = 1.22$. The intracavity pump is $|\psi_0|^2 = 0.95$, so that it is *below* threshold. (a) Cavity soliton formation. (b) FFT of the soliton, corresponding to a wide-span, low-threshold Kerr frequency comb.

to transform the θ coordinate to remove the group velocity motion by making the transformation $\theta \to \theta - \zeta_1 t \bmod [2\pi]$. When we make these transformations, and the spectrum is restricted to the neighborhood of $\ell = \ell_0$, so that $\zeta_n, n \geqslant 3$ can be neglected and so that $\Lambda_\ell^{\ell_m \ell_n \ell_p} \simeq 1$, then Eq. (7) becomes

$$\frac{\partial \mathcal{A}}{\partial t} = -\frac{1}{2}\Delta\omega_{\ell_0}\mathcal{A} - i\sigma\mathcal{A} + \frac{1}{2}\Delta\omega_{\ell_0}\mathcal{F}_0 - ig_0|\mathcal{A}|^2\mathcal{A} - i\frac{\zeta_2}{2}\frac{\partial^2 \mathcal{A}}{\partial\theta^2}. \quad (8)$$

This equation can be rewritten in the form of the normalized Lugiato-Lefever equation

$$\frac{\partial\psi}{\partial\tau} = -(1+i\alpha)\psi + i|\psi|^2\psi - i\frac{\beta}{2}\frac{\partial^2\psi}{\partial\theta^2} + F, \quad (9)$$

where the field envelope has been rescaled so that $\psi = (2g_0/\Delta\omega_{\ell_0})^{1/2}\mathcal{A}^*$ and the time has been rescaled so that $\tau = \Delta\omega_{\ell_0} t/2$. The dimensionless parameters of this normalized equation are the frequency detuning $\alpha = -2\sigma/\Delta\omega_{\ell_0}$, the dispersion $\beta = -2\zeta_2/\Delta\omega_{\ell_0}$, and the external pump $F = (2g_0/\Delta\omega_{\ell_0})^{1/2}\mathcal{F}_0^*$. This LLE with *periodic* boundary conditions is the *exact* counterpart of the modal expansion as long as higher-order dispersion and the variation of $\Delta\omega_\ell$ and $\Lambda_\ell^{\ell_m\ell_n\ell_p}$ in Eq. (2) can be neglected. Since the higher-order corrections can be calculated, it is always possible to check the validity of the LLE. 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 and its extensions when the bandwidth becomes large. 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 (solitons or Turing rolls) 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 $|\mathcal{A}|^2_{\rm th} = \Delta\omega_{\ell_0}/2g_0$, which exactly corresponds to $|\psi|^2_{\rm th} = 1$. Hence, we would expect ψ to be on the order of 1 in our theoretical analysis and numerical simulations. Note that the stationary intracavity field ψ_0 before comb generation can be obtained by setting all the derivatives to zero in Eq. (9). The dimensionless time can be rewritten as $t/2\tau_{\rm ph}$, where we recall that $\tau_{\rm ph}$ is the photon lifetime, which is typically a few microseconds in ultrahigh-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 α 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 β 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 interesting to note that the LLE formalism sheds new light on the role of dispersion on Kerr-comb formation: In Eq. (9) no comb generation can occur when the dispersion parameter β is null since ψ becomes independent of the azimuthal angle θ ("flat" solutions). The case of the generalized LLE in Eq. (7) is however less trivial to analyze in this regard. The overall dispersion has to be a relatively small parameter in all cases. 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 preferably not be too large ($\sim$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 [19,20].

Numerical simulations were performed using the split-step Fourier algorithm, which is commonly used in simulations of the one-dimensional (1D) 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. (9)] we have considered a calcium fluoride resonator with a radius $a = 2.5$ mm. The polar eigennumber of the TE-polarized pump mode is $\ell_0 = 14\,350$, corresponding to a wavelength of 1560.5 nm and $\omega_{\ell_0} = 2\pi \times 192.24$ THz in vacuum. The index of refraction is $n_0 = 1.43$. The resonator is critically coupled with a loaded quality factor $Q_0 = 3 \times 10^9$, corresponding to a central mode bandwidth of $\Delta\omega_{\ell_0} = \omega_{\ell_0}/Q \simeq 2\pi \times 64$ kHz. The free spectral range is equal to $\Delta\omega_{\rm FSR} = \zeta_1 = 2\pi \times 13.36$ 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(a) shows the formation of a single-peaked cavity soliton. This dissipative localized structure is obtained after subcritical pumping. The figure corresponds to a single pulse of width $\Delta T \simeq 500$ fs, circulating inside the cavity with a round-trip time $T = 2\pi/\Delta\omega_{\rm FSR} \simeq 75$ ps. In the frequency domain, this pulse consists of several tens of modelocked whispering-gallery modes, whose frequencies have been nonlinearly shifted so that they are equidistant, as shown in Fig. 2(b). In order to obtain a single soliton, it is necessary to lower the power so that it is below threshold and to reduce the magnitude of the anomalous dispersion so that it is closer to zero. 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 $|\beta|$.

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, where the evolution variable is time, and the conjugate (transverse) variable is the azimuthal angle. 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 without too much difficulty to include Rayleigh and Brillouin scattering [21]. 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 [22,23].

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