Nonadiabatic semiconductor laser rate equations for the large-signal, rapid-modulation regime

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The standard multimode rate equation for semiconductor lasers is based on the approximation that modal field shapes (if they change at all) depend on the instantaneous value of the time-dependent dielectric function. This is known as the adiabatic approximation. It will break down if the inverse of the modulation frequency approaches the photon round-trip time in the cavity. In this paper, we derive a criterion for the validity of the adiabatic approximation and find that it also involves the fractional modulation of the dielectric function, not just the photon round-trip time and the modulation frequency. Recognizing that present laser designs are starting to approach the limits of validity as set by our criterion, we study what can be done to get past that limit. We obtain corrections to the equations presently used by rederiving these equations from the time-dependent wave equation *without* discarding the time derivative of the dielectric function, an approximation made in every other derivation we have encountered. Retaining this time derivative introduces new terms into the usual equations. These terms correctly account for propagation delay-time effects and for nonadiabatic couplings between the modes. Surprisingly, the new terms alter only the source of photons to each mode. The usual rate equations are driven by a spontaneous emission term $R_\nu^{\rm sp}(t)$, which represents the rate at which photons are emitted spontaneously into the mode ν. In the rate equation derived here, the spontaneous emission term $R_\nu^{\rm sp}(t)$ is augmented by a term $\Xi_\nu(t)$ which counts photons that were earlier emitted spontaneously into other modes μ, accumulated and perhaps amplified there, and are now, because of the breakdown of the adiabatic approximation, leaking into the νth mode. Although casting the equations into this form makes sense from a physical point of view, it leads to great computational difficulties in solving the equations because $\Xi_\nu(t)$ refers explicitly to the past history of the laser. To overcome this practical problem, we provide an efficient and accurate algorithm for stepping the laser forward in time without having to retain history prior to the start of the present time step. Our method allows the equations to be solved with substantially the same computational effort as is normally expended in solving the conventional rate equations, and, moreover, provides error estimates at each step of the way.

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I. INTRODUCTION

All formulations of the rate equations and large-modulation traveling-wave equations governing semiconductor lasers assume that $\omega_{\rm max}$, the maximum frequency at which the laser is modulated, is small compared to the inverse of T_p, the photon round-trip time within the laser cavity. (For distributed feedback lasers, the equivalent assumption is that the maximum modulation frequency is appreciably less than $\Delta\omega$, the frequency spacing between adjacent longitudinal modes.) Within both formulations, the modes in which the electric field is expanded depend on the instantaneous form of a time-dependent dielectric function. This is an adiabatic description of the field. We shall show that under certain well-defined conditions, ignoring the (nonadiabatic) couplings between these adiabatic modes destroys the validity of the governing equation. Although the general belief is that the maximum modulation frequency for which the governing equations can be used is $\omega_{\rm max}T_p \ll 2\pi$ or $\omega_{\rm max}/\Delta\omega \ll 1$, we find that the criterion is more complicated than this. Consequently, there may be, depending on the length of the laser and the fractional change in its dielectric constant during modulation, important corrections to the equations presently in use. In this paper, we derive rate equations that retain the nonadiabatic couplings to all orders. We also provide an accurate efficient numerical algorithm for dealing with the new rate equations which, as formulated, depend on the past history of the laser. They would otherwise be computationally prohibitive to solve.

Before proceeding further, it is useful to understand how the interplay between the maximum modulation frequency, the fractional change in the dielectric constant, and the breakdown of the adiabatic assumption comes about. The adiabatic method uses a time-independent equation, e.g., the Helmholtz equation, to calculate the field in a system where the dielectric function depends parametrically on time. In terms of a Huygens' principle description of wave propagation, the validity of the adiabatic method depends on the local dielectric function undergoing only a small fractional change during the time that light leaving some neighborhood returns to that same neighborhood. Satisfying this criterion puts an upper limit on the rate at which the dielectric function can change.

To develop this idea somewhat more quantitatively, consider the dielectric function as a sum of two parts, a static and a dynamic:

$$\varepsilon_\omega(r,t)=\varepsilon_s(r)+\varepsilon_d(r,t).$$

In the laser, the dynamic part is much smaller than the static part. The characteristic time for light to return to its starting point is T_p, the photon round-trip time in the cavity. The fractional change in the dielectric constant during this time will be

$$\frac{\delta\varepsilon_\omega}{\varepsilon_\omega(r,t)} \approx \frac{1}{\varepsilon_\omega} T_p \frac{\partial \varepsilon_d}{\partial t} \approx \frac{\varepsilon_d}{\varepsilon_\omega} \omega_{\max} T_p$$

where we have assumed a maximum modulation frequency of $\omega_{\max}$. Thus, the criterion for validity of the adiabatic approximation is that the product of two dimensionless factors, one expressing the fractional change in dielectric constant and the other expressing the speed of modulation, should be small. ''How small'' is the question we must answer. The quantitative answer, which is derived later in the paper, is contained in the following equation:

$$\Omega\, \omega_{\max} T_p \ll \frac{(2\pi)^2}{\omega T_p}\left(1 - \frac{\omega_{\max} T_p}{2\pi}\right). \tag{1.1a}$$

The quantity Ω resembles the term $\varepsilon_d/\varepsilon_\omega$. Actually, it is the ratio of an off-diagonal matrix element of ε_d to a diagonal element of the group dielectric function, that is,

$$\Omega \equiv \frac{\langle E_\mu | \varepsilon_d | E_\nu \rangle}{\langle E_\nu | \varepsilon + (\omega/2)(\partial\varepsilon/\partial\omega) | E_\nu \rangle}, \quad \mu \neq \nu. \tag{1.1b}$$

ω is the laser optical frequency. The last factor on the right-hand side of Eq. (1.1a) causes the adiabatic approximation, as expected, to break down completely at $\omega_{\max} T_p = 2\pi$ where the inequality can never be satisfied. What comes perhaps as a surprise is the presence of the small factor $(\omega T_p)^{-1}$ on the right of Eq. (1.1a). This factor gives rise to the severest restriction on the size of the dimensionless product $\Omega\omega_{\max} T_p$.

While the criterion (1.1a) is easily satisfied for two-dimensional (2D) laser simulations where the field confinement in the *x,y* plane is tight enough to make T_p small [1], it is only marginally satisfied for 3D lasers at present and will be violated if we increase modulation frequency, cavity length, or strength of modulation. As an example of the present situation, consider a laser operating at 1.5 μm with a modulation frequency of 20 GHz, a cavity length of 300 μm and a group index of 3.5. Suppose that Ω is only 10^{-3}. The left side of Eq. (1.1a) is then smaller than the right by only a factor of 4. Doubling the length of the laser makes the left side slightly exceed the right. Doubling the modulation frequency instead makes the left side slightly larger than half of the right. Thus, although the violation of the adiabatic approximation is not an acute concern at present, the quest for higher modulation rates and/or greater modulation depths may make the nonadiabatic corrections essential.

To obtain the nonadiabatic corrections, we must retain terms containing $\partial\varepsilon_d/\partial t$ in our equations, terms that are universally dropped on the way from the time-dependent wave equation to the rate equations for the photon number $S_\nu(t)$. The photon number is defined by the role it plays in Eq. (1.3) below, and the rate equation governing it takes the form:

$$\frac{dS_\nu}{dt} = \left(G_\nu - \frac{1}{\tau_\nu}\right) S_\nu + R_\nu^{\text{sp}}. \tag{1.2}$$

G_ν and $1/\tau_\nu$ are the modal gain and the modal loss. R_ν^{sp} is the rate of spontaneous emission into the mode. As the laser evolves forward in time, the gain, the loss, and the spontaneous emission into each mode have to be reevaluated. These terms depend on the dielectric function which is itself changing as the laser evolves. However, evaluation of the dielectric function will not concern us here: a substantial literature [1] exists on this point and instead we shall assume the dielectric function is known. This allows us to focus solely on the equations that the field must satisfy.

Assume that the electric field in the laser can be expanded in the form

$$E(r,t) = \phi(x,y) \sum_\nu \sqrt{S_\nu(t)}\, e^{-i\int_0^t d\tau\, \omega_\nu(\tau)} Z_\nu(z,t) + \text{c.c.} \tag{1.3}$$

If $\phi(x,y)Z_\nu(z,t)$ is written as

$$E_\nu(r,t) \equiv \phi(x,y) Z_\nu(z,t) = R_\nu(r,t) e^{-i\zeta_\nu(r,t)} \tag{1.4}$$

[where $\omega_\nu(t)$, $R_\nu(r,t)$, and $\zeta_\nu(r,t)$ are real] the νth mode in Eq. (1.4) will have a local frequency

$$\omega_\nu(r,t) = \omega_\nu(t) + \frac{d}{dt}\zeta_\nu(r,t). \tag{1.5}$$

The sum over modes in Eq. (1.3) allows one or another to become dominant as the laser moves from one point on the gain spectrum to another. The flexibility of each individual mode $E_\nu(z,t)$ allows it to respond to changes in the spatial form of the dielectric constant as the laser is modulated.

The derivation to be presented here starts by inserting Eq. (1.3) into the time-dependent wave equation with sources, and solving the resulting equations using the time-dependent Green's function $G(r,t;r',t')$. The form of the Green's function is remarkably simple when the adiabatic approximation is valid. An equivalent statement of the adiabatic approximation is that a photon, started in one time-dependent mode, remains in that same mode as the system evolves. The criterion for the validity of that approximation is well known for quantum-mechanical systems. We apply that same criterion to the laser system to find out when we can use this simplified form of Green's function. This is how we obtained Eq. (1.1). However, without assuming the validity of the adiabatic approximation, we do use the full Green's function to provide a solution in much the same way as Henry did in using $G_\omega(z,z')$ in the static case [2]. We then construct an expression for the field-field correlation function and perform an ensemble average over the random spontaneous emission events that give rise to the field. This allows us to construct a rate equation for the photon number and leads to expressions for the spectrum of emitted power. The rate equation reduces to the standard form (1.2) when the adiabatic approximation is valid. When it is not, use of the full Green's function leads to a new rate equation in which the spontaneous emission term $R_\nu^{\text{sp}}(t)$ is augmented by a term $\Xi_\nu(t)$. $\Xi_\nu(t)$ counts photons that were emitted spontaneously into other modes μ at an earlier time, have been stored or amplified there, and are now, because of the breakdown of the adiabatic approximation, leaking into the νth mode. The effect of this photon leakage is expected to be largest for the side modes, and to act in the direction of increasing their amplitude relative to that of the main mode, i.e., to decrease the side-mode suppression ratio. This will come about because leakage into the side modes of even a small fraction of the many photons in the lasing mode will greatly enhance the source of photons to the side modes. Conversely, the side modes will not contain enough photons to act effectively as a source to the lasing mode.

There are some limitations to the formalism. It is based on a first-order dielectric function. That is, the polarization response of the medium (whose carrier distributions are assumed known) is taken to be proportional to the first power of the electric field. This precludes study of, e.g., four-wave mixing and other nonlinear phenomena. Secondly, modulation rates are assumed slow on the time scale of polarization decay. The polarization is governed by the conventional dielectric response function rather than treated as a dynamic system in its own right. This precludes study of certain ultrafast phenomena. Thirdly, the formalism is not well suited to the study of noise and fluctuation effects. These are usually treated as small-signal responses to stochastic forces and are more appropriately studied in a formalism not specifically tailored to large-signal response.

This paper is arranged as follows. Section II consists of two parts. The first leads from Maxwell's equations to the wave equation in the time domain and is not new. It does allow us to reiterate some ideas we use later. The second part is new. In it, we solve the time-domain wave equation in terms of adiabatic modes oscillating at adiabatic time-dependent frequencies. We use a generalized eigenvalue equation to define the modes and give a criterion for determining their adiabatic frequencies. The nonadiabatic transition operator is defined here and the equations governing the Green's function, including nonadiabaticity, are derived. Section III is motivated by the fact that the sources of the field, and therefore the field itself, are stochastic. There are several ways to deal with this. We choose to use the Green's function solution to express the field-field correlations in terms of time-domain source-source correlations. This allows us to derive a nonadiabatic rate equation that reduces to the standard rate equation at low modulation frequencies. In Sec. IV, we relate the time-domain source-source correlation function to the frequency-domain source-source correlation function, a quantity that Henry [2] has already worked out. Section V presents the numerical algorithm that makes the method practical for doing calculations. A short summary concludes the paper in Sec. VI. The adiabatic criterion (1.1) is derived in Appendix A. Numerical results will appear separately.

II. GREEN'S FUNCTION SOLUTION IN THE TIME DOMAIN

A. Background

In a dielectric medium with negligible magnetic properties, the constitutive equations are

$$D(r,t)=E(r,t)+4\pi[P(r,t)+K(r,t)], \tag{2.1a}$$

$$H(r,t)=B(r,t). \tag{2.1b}$$

P and K are components of the polarization in the dielectric medium. P is the response of the medium to the electric field. Taking it to be isotropic, local, and causal,

$$P(r,t)=\int_{-\infty}^{t}\chi(r,t,t')E(r,t')dt'. \tag{2.1c}$$

χ is the first-order polarization response kernel. K represents the contribution to D arising from spontaneous fluctuations of the medium. This point of view was taken by Landau and Lifshitz [3] and later served as the starting point for Henry's work on noise in the steady-state laser [2].

The space and time dependence of the fields satisfy Maxwells equations with charge density and current set to zero because at optical frequencies there is no appreciable accumulation of charge or current. These equations can be combined in the usual way, i.e., making use of the constitutive equations (2.1) and dropping (as is always done [4]) the $\nabla(\nabla\cdot E)$ term, which arises from the vector identity $\nabla\times\nabla\times E=\nabla(\nabla\cdot E)-\nabla^2 E$. The result is the wave equation

$$\nabla^2E(r,t)-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\left(E(r,t)+4\pi\int_{-\infty}^{t}\chi(r,t,t')E(r,t')dt'\right)=\frac{4\pi}{c^2}\frac{\partial^2}{\partial t^2}K(r,t). \tag{2.2}$$

If the system were truly time-translationally invariant, then the polarization response would depend on t and t' only via the combination $\tau\equiv t-t'$. In that case, the induced polarization could have been written as

$$P(r,t)=\int_0^{\infty}\chi(r,\tau)E(r,t-\tau)d\tau. \tag{2.3}$$

The kernel $\chi(\tau)$ has a limited range: polarization induced by a pulse of electric field decays away after a short time due to collisions and dephasing. That short time is of the order of 10^{-13} seconds [5]. However, the system is *not* time-translationally invariant because the response kernel depends on the local density of carriers in the system, and that density can be time dependent. The shortest time scale associated with this dependence is set by the highest frequency at which the laser can be modulated. At the present time, that frequency does not exceed 40 GHz. This corresponds to a time of 2.5×10^{-11} seconds or longer. This is very slow on the time scale of the polarization decay, and so, on the faster time scale, the system is *effectively* time-translationally invariant. None the less, there is still a secular variation in χ, and so instead of Eq. (2.3), we must write

$$P(r,t)=\int_0^{\infty}\chi(r,t,\tau)E(r,t-\tau)d\tau,$$

where the t dependence of χ arises solely through the time dependence of the carrier density on which χ depends. [A similar point of view has been taken in Eq. (7) of [6].] In terms of the dielectric response kernel

$$\varepsilon(r,t,\tau)=\delta(\tau)+4\pi\chi(r,t,\tau),$$

Eq. (2.3) becomes

$$\nabla^2 E(r,t) - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\int_0^\infty \varepsilon(r,t,\tau)E(r,t-\tau)d\tau = \frac{4\pi}{c^2}\frac{\partial^2}{\partial t^2}K(r,t). \quad (2.4)$$

The one-sided Fourier transform of ε,

$$\varepsilon_\omega(r,t) = \int_0^\infty \varepsilon(r,t,\tau)e^{+i\omega\tau}d\tau, \quad (2.5)$$

is the frequency-dependent dielectric function in a time-dependent medium. It depends on r and t via the composition and carrier density. If there is gain or loss locally, then ε_ω has a local negative or positive imaginary part [7].

B. Development

Assume that the field has the form

$$E(r,t) = \sum_\nu a_\nu(t)e^{-i\int_0^t d\tau\, \omega_\nu(\tau)}E_\nu(r,t) + \text{c.c.} \quad (2.6)$$

Inserting Eq. (2.6) into Eq. (2.4) will result in equations for the $a_\nu(t)$. The equations depend on the choice of $\omega_\nu(t)$ and $E_\nu(r,t)$ but that choice can be left open for now. The second term of Eq. (2.4) becomes the integral of

$$\frac{\partial^2}{\partial t^2}[U_\nu(r,t,\tau)\Phi_\nu(t-\tau)] = \ddot{U}_\nu\Phi_\nu + 2\dot{U}_\nu\dot{\Phi}_\nu + U_\nu\ddot{\Phi}_\nu, \quad (2.7)$$

where

$$U_\nu(r,t,\tau) \equiv \varepsilon(r,t,\tau)a_\nu(t-\tau)E_\nu(r,t-\tau), \quad (2.8a)$$

$$\Phi_\nu(t-\tau) \equiv e^{-i\int_0^{t-\tau}\omega_\nu(t')dt'}. \quad (2.8b)$$

Note that

$$\dot{\Phi}_\nu = -i\omega_\nu(t-\tau)\Phi_\nu(t-\tau),$$

$$\ddot{\Phi}_\nu = -[i\dot{\omega}_\nu(t-\tau) + \omega_\nu^2(t-\tau)]\Phi_\nu(t-\tau).$$

$U_\nu(r,t,\tau)$ is a slowly varying function of t, oscillating at best with a frequency ω_{mod}, the frequency at which the laser is modulated. We shall use 50 GHz as a frequency we would like to reach. $\Phi_\nu(t)$, on the other hand, oscillates at the modal frequency ω_ν, which for a laser with a free-space wavelength of 1.5 μm is 4000 times larger. Thus, the term in $\ddot{U}$ is smaller than the term in $\ddot{\Phi}$ by a factor of 10^{-7} and can be dropped, leaving an expression we rewrite as

$$\frac{\partial^2}{\partial t^2}U_\nu\Phi_\nu = -\Phi_\nu(t)[\omega_\nu^2(t-\tau)U_\nu + i\dot{\omega}_\nu(t-\tau)U_\nu + 2i\omega_\nu(t-\tau)\dot{U}_\nu]\Phi_\nu(t-\tau)/\Phi_\nu(t). \quad (2.9)$$

The last factor is

$$\Phi_\nu(t-\tau)/\Phi_\nu(t) = e^{+i\int_{t-\tau}^t \omega_\nu(t')dt'}. \quad (2.10)$$

The τ integration in Eq. (2.4) cuts off at values of $\tau \approx \tau_{\text{pol}} \approx 10^{-13}$ seconds because of the short range of the dielectric kernel ε. Take advantage of this by expanding $\omega_\nu(t')$ in Eq. (2.10) to first order in $(t'-t)$,

$$\int_{t-\tau}^t \omega_\nu(t')dt' \approx \int_{t-\tau}^t [\omega_\nu(t) + (t'-t)\dot{\omega}_\nu(t)]dt' = \tau\omega_\nu(t) - \tfrac{1}{2}\tau^2\dot{\omega}_\nu(t). \quad (2.11)$$

The largest value of each term in Eq. (2.11) is at τ_{pol} where the integral cuts off. To estimate the size of each term, we write

$$\omega_\nu(t) = \omega_\nu^0 + \Delta\omega_\nu(t),$$

where ω_ν^0 is the nominal optical frequency of the νth mode ($\approx 2\pi\times 2\times 10^{14}\,\text{sec}^{-1}$) and $\Delta\omega_\nu$ is the frequency shift, or chirp, the laser might encounter during operation. Only during extreme conditions will the fractional chirp $\Delta\omega_\nu/\omega_\nu$ become as large as 10^{-2}. If the laser is being modulated at a frequency ω_{mod}, then $\dot{\omega}_\nu$ is of order

$$\dot{\omega}_\nu \approx \omega_{\text{mod}}\Delta\omega_\nu \lesssim 10^{-2}\omega_{\text{mod}}\omega_\nu.$$

On this basis, the first term in Eq. (2.11) could be of order 10^2 while the second is of order 10^{-2}. The appropriate evaluation of Eq. (2.10) for use within the integrand of Eq. (2.4) is

$$\Phi_\nu(t-\tau)/\Phi_\nu(t) = e^{+i\tau\omega_\nu(t)}\left(1 - \frac{i}{2}\tau^2\dot{\omega}_\nu(t)\right). \quad (2.12)$$

The second term can be dropped provided the modulation frequency satisfies a condition similar to Eq. (1.1) with the much shorter polarization decay time τ replacing the round-trip time T_p. At higher modulation frequencies, it would be better to treat the polarization as a dynamic system. We can also use the short range of the dielectric kernel to expand the terms within the square brackets in Eq. (2.9) in powers of τ. For the first term, the appropriate expansion terminates at first order:

$$\omega_\nu^2(t-\tau)U_\nu(r,t,\tau) = \varepsilon(r,t,\tau)\left(\omega_\nu^2(t)a_\nu(t)E_\nu(t) - \tau\frac{\partial}{\partial t}\omega_\nu(t)^2 a_\nu(t)E_\nu(t)\right). \quad (2.13a)$$

The second and third terms in the square brackets of Eq. (2.9) are already smaller than the first by a factor of $\approx$4000, and so for them, the zeroth-order expansion is adequate:

$$\dot{\omega}_\nu(t-\tau)U_\nu(r,t,\tau) + 2\omega_\nu(t-\tau)\dot{U}_\nu(r,t,\tau) = \dot{\omega}_\nu(t)\varepsilon(r,t,\tau)a_\nu(t)E_\nu(r,t) + 2\omega_\nu(t)\frac{\partial}{\partial t}(\varepsilon a_\nu E_\nu). \quad (2.13b)$$

As was the case for Eq. (2.12), the higher-order terms dropped from Eq. (2.13) can be shown to be small enough to ignore Thus, Eq. (2.9) becomes

$$\frac{\partial^2}{\partial t^2}U_\nu\Phi_\nu=-e^{-i\int_0^t\omega_\nu(t')dt'}\Bigg[\varepsilon(r,t,\tau)\Bigg(\omega_\nu^2 a_\nu E_\nu-\tau\frac{\partial}{\partial t}(\omega_\nu^2 a_\nu E_\nu)+i\dot\omega_\nu a_\nu E_\nu+2i\omega_\nu\frac{\partial}{\partial t}a_\nu E_\nu\Bigg)+2i\dot\varepsilon(r,t,\tau)\omega_\nu a_\nu E_\nu\Bigg]e^{+i\tau\omega_\nu(t)}. \quad (2.14)$$

The only τ-dependent quantities appearing in Eq. (2.14) are those whose τ dependence has been indicated explicitly. The τ integration in Eq. (2.4) can be carried out by using Eq. (2.5). Three types of term appear:

$$\int_0^\infty\varepsilon(r,t,\tau)e^{+i\tau\omega_\nu(t)}d\tau=\varepsilon_{\omega_\nu(t)}(r,t)\equiv\varepsilon_\nu(r,t), \quad (2.15a)$$

$$\int_0^\infty\varepsilon(r,t,\tau)e^{+i\tau\omega_\nu(t)}\tau\,d\tau=-i\frac{\partial}{\partial\omega_\nu}\varepsilon_\nu(r,t), \quad (2.15b)$$

$$\int_0^\infty\dot\varepsilon(r,t,\tau)e^{+i\tau\omega_\nu(t)}d\tau=\dot\varepsilon_\nu(r,t). \quad (2.15c)$$

The overdot on $\dot\varepsilon(r,t,\tau)$ denotes the derivative with respect to t. The overdot on $\dot\varepsilon_\nu(r,t)$ denotes the time derivative of $\varepsilon_\omega(r,t)$ evaluated at $\omega=\omega_\nu(t)$. Later, we shall need the full time derivative of $\varepsilon_\nu(r,t)$, taking into account that ω_ν, the frequency of evaluation, may itself be time dependent. For this, we shall use the symbol $\partial/\partial t$ and in that case,

$$\frac{\partial}{\partial t}\varepsilon_\nu(r,t)\equiv\dot\varepsilon_\nu(r,t)+\dot\omega_\nu\frac{\partial\varepsilon_\nu}{\partial\omega_\nu}. \quad (2.16)$$

Equation (2.4) becomes

$$\sum_\nu e^{-i\int_0^t\omega_\nu(t')dt'}\Bigg[\nabla^2 a_\nu E_\nu+k_\nu^2 a_\nu E_\nu+iK_\nu^2\frac{\partial}{\partial t}a_\nu E_\nu+\frac{i}{c^2}\Bigg(\frac{\partial\omega_\nu^2}{\partial t}\frac{\partial\varepsilon_\nu}{\partial\omega_\nu}+\dot\omega_\nu\varepsilon_\nu+2\omega_\nu\dot\varepsilon_\nu\Bigg)a_\nu E_\nu\Bigg]=F(r,t), \quad (2.17)$$

where we have defined

$$k_\omega^2(r,t)=\frac{\omega^2}{c^2}\varepsilon_\omega(r,t), \quad (2.18a)$$

$$k_\nu^2=[k_\omega^2]_{\omega=\omega_\nu(t)}, \quad (2.18b)$$

$$K_\nu^2(r,t)=\frac{2\omega_\nu}{c^2}\left(\varepsilon_\nu+\frac{\omega_\nu}{2}\frac{\partial\varepsilon_\nu}{\partial\omega_\nu}\right) \quad (2.18c)$$

$$=\left[\frac{\partial}{\partial\omega}k_\omega^2(r,t)\right]_{\omega=\omega_\nu(t)}, \quad (2.18d)$$

$$F(r,t)\equiv\frac{4\pi}{c^2}\frac{\partial^2}{\partial t^2}K(r,t)=\frac{4\pi}{c^2}\frac{\partial}{\partial t}j_{\rm sp}(r,t). \quad (2.18e)$$

Further progress in obtaining equations for the $a_\nu(t)$ requires making a choice for the modal fields $E_\nu(r,t)$ and the modal frequencies $\omega_\nu(t)$. The only necessary condition is that the fields be complete enough to expand any electric field in the interior of the laser. The choice made here is to have the fields satisfy

$$[\nabla^2+k_\nu^2(r,t)-\lambda_\nu(t)K_\nu^2(r,t)]E_\nu(r,t)=0 \quad (2.19a)$$

plus outgoing-wave boundary conditions on the surface of the laser. The normalization will be taken to be

$$\langle E_\nu K_\nu^2 E_\nu\rangle=1, \quad (2.19b)$$

where $\langle\cdots\rangle$ denotes integration over the volume of the laser. This is a generalized eigenvalue equation with λ_ν being the eigenvalue. The real frequency $\omega_\nu(t)$ will be determined by the condition that λ_ν be purely imaginary at each instant: i.e., that

$$\mathrm{Re}[\lambda_\nu(\omega_\nu)]=0. \quad (2.19c)$$

A useful consequence of Eq. (2.19a) is that, up to terms linear in k_ω^2, the modes satisfy the following orthogonality relation:

$$\langle E_\mu(t)K_\nu^2(t)E_\nu(t)\rangle=\delta_{\mu\nu}. \quad (2.19d)$$

Modal fields $\hat E_\mu(r,t)$ and $\tilde E_\mu(r,t)$ are defined as

$$\hat E_\mu(r,t)\equiv e^{-i\int_0^t\omega_\mu(t')dt'}E_\mu(r,t), \quad (2.20a)$$

$$\tilde E_\mu(r,t)\equiv e^{+i\int_0^t\omega_\mu(t')dt'}E_\mu(r,t). \quad (2.20b)$$

We multiply Eq. (2.17) by $\tilde E_\mu(r,t)$ and integrate over the laser volume. The result is

$$\lambda_\mu(t)a_\mu(t)+i\frac{d}{dt}a_\mu(t)+i\sum_\nu T_{\mu\nu}(t)a_\nu(t)=F_\mu(t), \quad (2.21)$$

where

$$F_\mu(t)\equiv\langle E_\mu(t)F(t)\rangle e^{i\int_0^t\omega_\mu(\tau)d\tau}, \quad (2.22a)$$

$$T_{\mu\nu}(t)\equiv t_{\mu\nu}(t)e^{i\int_0^t[\omega_\mu(\tau)-\omega_\nu(\tau)]d\tau}, \quad (2.22b)$$

$$t_{\mu\nu}(t)\equiv\langle E_\mu K_\nu^2\dot E_\nu\rangle+\frac{1}{c^2}\left\langle E_\mu\left(\dot\omega_\nu\varepsilon_\nu+2\omega_\nu\dot\varepsilon_\nu+\frac{\partial\varepsilon_\nu}{\partial\omega_\nu}\frac{\partial\omega_\nu^2}{\partial t}\right)E_\nu\right\rangle. \quad (2.22c)$$

Not all of the terms in $t_{\mu\nu}(t)$ are equally important. To extract the important ones, first evaluate $\langle E_\mu K_\nu^2 \dot{E}_\mu \rangle$ for the case $\mu=\nu$ by differentiating the normalization condition (2.19b) with respect to t:

$$\langle E_\nu K_\nu^2 \dot{E}_\nu \rangle = -\tfrac{1}{2} \left\langle E_\nu \left(\frac{\partial}{\partial t} K_\nu^2 \right) E_\nu \right\rangle. \tag{2.23}$$

For $\mu \neq \nu$, differentiate Eq. (2.19a) with respect to t:

$$(\nabla^2 + k_\nu^2 - \lambda_\nu K_\nu^2)\dot{E}_\nu + \left(\frac{\partial}{\partial t} k_\nu^2 - \dot{\lambda}_\nu K_\nu^2 - \lambda_\nu \frac{\partial}{\partial t} K_\nu^2 \right) E_\nu = 0.$$

Multiplying by E_μ and integrating over r gives

$$\langle E_\mu (k_\nu^2 - k_\mu^2 - \lambda_\nu K_\nu^2 + \lambda_\mu K_\mu^2) \dot{E}_\nu \rangle + \left\langle E_\mu \left(\frac{\partial}{\partial t} k_\nu^2 - \lambda_\nu \frac{\partial}{\partial t} K_\nu^2 \right) E_\nu \right\rangle = 0. \tag{2.24}$$

The orthogonality condition was based on the assumption that k_ω^2 was adequately represented as being a linear function of ω over the frequency range spanned by the various frequencies ω_μ. To this same order of approximation, we have

$$k_\nu^2 - k_\mu^2 = (\omega_\nu - \omega_\mu) K_\nu^2,$$

$$K_\nu^2 - K_\mu^2 = 0.$$

This allows us to rearrange Eq. (2.24) as

$$\langle E_\mu K_\nu^2 \dot{E}_\nu \rangle = \frac{\langle E_\mu ((\partial/\partial t) k_\nu^2 - \lambda_\nu (\partial/\partial t) K_\nu^2) E_\nu \rangle}{\tilde{\omega}_\mu - \tilde{\omega}_\nu}, \tag{2.25}$$

where the complex frequencies in the denominator are defined by

$$\tilde{\omega}_\nu(t) \equiv \omega_\nu(t) - \lambda_\nu(t). \tag{2.26}$$

We can now make the following order-of-magnitude estimates:

(a) $\dot{\omega}_\nu \lesssim 10^{-2} \omega_{\max} \omega_\nu$,

(b) $\dot{\varepsilon}_\nu \lesssim -2 \times 10^{-2} \omega_{\max} \varepsilon_\nu$,

(c) $\omega \partial\varepsilon/\partial\omega \approx \sigma\varepsilon$,

(d) $K_\nu^2 \approx k_\nu^2/\omega_\nu$,

(e) $\langle E_\nu (\cdots) E_\mu \rangle \approx (\cdots)/K_\nu^2$.

Estimate (a) was made earlier, after Eq. (2.11). Estimate (b) follows from the fact that, in a Fabry-Pérot laser of length L, the quantity $\omega^2 \varepsilon_\omega L^2/c^2$ is almost invariant with respect to frequency. Estimate (c), in which σ is of the order 0.1–0.3, is empirically true for semiconductor laser dielectrics in the optical and infrared. For order-of-magnitude purposes, $\sigma \approx 1$. Estimate (d) follows from the definitions (2.18). Estimate (e) follows from the normalization condition (2.19b). Using these estimates, each of the three last terms in Eq. (2.22c) is of order $< 10^{-2} \omega_{\max}$, as is Eq. (2.23). In Eq. (2.25), the second term is of order λ_ν/ω_ν times the first. It will later turn out that $i\lambda_\nu = (G_\nu - 1/\tau_\nu)/2$, and so the second term is utterly negligible compared to the first. The first term is of order $\omega_\nu/(\tilde{\omega}_\nu - \tilde{\omega}_\mu) \approx 10^3$ times larger than any of the other terms in $t_{\mu\nu}$, which allows us to drop the other terms. Using a notation similar to Eq. (2.16), we transform that first term to

$$\frac{\partial}{\partial t} k_\nu^2 = \frac{\omega_\nu^2}{c^2} \dot{\varepsilon}_\nu + \dot{\omega}_\nu \frac{\partial}{\partial \omega} k_\nu^2 = \frac{\omega_\nu^2}{c^2} \dot{\varepsilon}_\nu + \dot{\omega}_\nu K_\nu^2.$$

The term in K_ν^2 vanishes in the matrix element because of Eq. (2.19d). Thus, instead of Eq. (2.22c), we have

$$t_{\mu\nu}(t) = \frac{(\omega_\nu/c)^2 \langle E_\mu | \dot{\varepsilon}_\nu | E_\nu \rangle}{\tilde{\omega}_\mu - \tilde{\omega}_\nu} (1 - \delta_{\mu\nu}). \tag{2.27}$$

The operator $t_{\mu\nu}(t)$ is the source of nonadiabatic transitions between the modes. Its size is proportional to the rate at which the dielectric function is changing, to the shape of $\dot{\varepsilon}$, via the matrix element between modes, and it is inversely proportional to the spacing between mode frequencies.

Return to Eq. (2.21) for $a_\mu(t)$. We write the solution as

$$a_\mu(t) = \frac{1}{i} \sum_\kappa \int_{-\infty}^{t} dt' \, g_{\mu\kappa}(t,t') F_\kappa(t') \tag{2.28}$$

and find that the $g_{\mu\kappa}(t,t')$ must satisfy the following set of coupled equations and boundary conditions:

$$\lambda_\mu(t) g_{\mu\kappa}(t,t') + i \frac{\partial}{\partial t} g_{\mu\kappa}(t,t') + i \sum_{\nu \neq \mu} T_{\mu\nu}(t) g_{\nu\kappa}(t,t') = 0, \tag{2.29a}$$

$$g_{\mu\kappa}(t',t') = \delta_{\mu\kappa}. \tag{2.29b}$$

The $E(r,t)$ field can be reconstructed using Eqs. (2.6), (2.28), and (2.22a). The result is of the form

$$E(r,t) = \int d^3 r_1 \int_{-\infty}^{t} dt_1 G(r,t,;r_1,t_1) F(r_1,t_1) + \text{c.c.} \tag{2.30}$$

with

$$G(r,t;,r_1,t_1) = \frac{1}{i} \sum_{\mu\nu} \hat{E}_\mu(r,t) g_{\mu\nu}(t,t_1) \tilde{E}_\nu(r_1,t_1). \tag{2.31}$$

The diagonal elements of the transition matrix $T_{\mu\nu}$ vanish because of Eq. (2.27). The off-diagonal elements (2.22b) oscillate rapidly, with the lowest frequency $\omega_\nu - \omega_{\nu+1}$ being $\approx 2\pi/T_p$, where T_p is the photon round-trip time within the cavity. This round-trip time is of the order of 7×10^{-12} seconds, corresponding to $\approx$150 GHz, far faster than lasers now can be modulated. The adiabatic approximation assumes that, because of the disparity of time scales, the off-diagonal elements of $g_{\nu\kappa}$ never have a chance to build up appreciably from their initial value of zero. Thus, in the adiabatic approximation, $g_{\mu\nu}$ is diagonal,

$$g_{\mu\nu}(t,t')=e^{i\int_{t'}^{t}\lambda_\mu(\tau)d\tau}\delta_{\mu\nu}, \tag{2.32a}$$

and the Green's function is

$$G(r,t;r',t')=\frac{1}{i}\sum_\nu E_\nu(r,t)e^{-i\int_{t'}^{t}\tilde{\omega}_\nu(\tau)d\tau}E_\nu(r',t'). \tag{2.32b}$$

As the inverse of the modulation frequency approaches the photon round-trip time, one expects radiation launched into one mode to leak into other modes. To study the issue quantitatively, we note that the mathematics used in Eqs. (2.20)–(2.22) is almost identical to that used to discuss adiabatic perturbations in quantum mechanics. In Appendix A, we use the same methods to study when the approximation (2.32a) is justified. When it is not justified, one must numerically integrate Eqs. (2.29a) and (2.29b) or something equivalent (see Sec. V).

Nothing has been said about how to solve the eigenvalue equation (2.19a). This equation, or closely related ones, is routinely solved in every study of the one-dimensional (z) laser after separating the transverse field dependence from the longitudinal. Traveling-wave methods [8–12], transfer-matrix methods in which uniform sections of the laser are coupled [13–15], spatial Green's function techniques [16,17], tooth-by-tooth integration schemes [18], variational methods [19], and transfer-matrix tooth-by-tooth methods [20,21] are routinely used and could be used here as well.

There is no need to work with the full Green's function if the structure supports only a single transverse mode. In that case, it is sufficient to approximate $E_\nu(r,t)$ by

$$E_\nu(r,t)\approx\phi(x,y)Z_\nu(z,t), \tag{2.33}$$

which is equivalent to approximating the full Green's function by

$$G(r,t;r',t')\approx\phi(x,y)G(z,t;z',t')\phi(x',y'). \tag{2.34}$$

The details of the equations for $\phi(x,y,t)$ and $Z_\nu(z,t)$ are easily worked out. In particular, the equation for $Z_\nu(z,t)$ that results from projecting Eq. (2.17) onto $\phi(x,y)^2$ can stand alone as the optical part of a one-dimensional (z,t) laser modeling program. Because of computational efficiency (see Sec. V) this could serve as an alternative to the traveling-wave (z,t) description, which seems, with one exception [22], to have been applied only in the small-signal regime.

III. THE FIELD-FIELD CORRELATION FUNCTION AND THE NONADIABATIC RATE EQUATION

Direct evaluation of Eq. (2.30) is not useful because of the stochastic nature of the source term $S(r,t)$. Averaging the equations over the ensemble of realizations of the source does not help because that average, denoted as $\langle S(r,t)\rangle$, vanishes, and hence $\langle E(r,t)\rangle$ vanishes too. The way to proceed is to recognize that the information needed from the field $E(r,t)$ is its power spectrum. This can be obtained from the field-field correlation function, namely, $\langle E(r,t+\tau)E(r,t)\rangle$ [23]. The Green's function solution (2.30) makes it possible to evaluate the field-field correlation function in terms of the nonvanishing source-source correlation function.

The correlation function $\psi(\tau,r,t)$ from which the power spectrum can be derived is not an instantaneous function of the fields but is rather an average, taken over a time period T large enough to kill any interference between the various frequency components of the fields [23]. Its precise definition is

$$\psi(\tau,r,t)\equiv\frac{1}{T}\int_{t-T/2}^{t+T/2}dt'E(r,t'+\tau/2)E(r,t'-\tau/2). \tag{3.1a}$$

From the definition, $\psi(\tau)$ is an even function of τ and in what follows, we shall consider τ to be non-negative. Equation (3.1a) can also be written as

$$\psi(\tau,r,t)\equiv\frac{1}{T}\int_{t-T/2}^{t+T/2}dt'E(r,t'+\tau)E(r,t')+O\left(\frac{\tau}{T}E^2\right). \tag{3.1b}$$

This will prove to be more convenient and, since our final working equations will be derived in the limit $\tau\rightarrow0$, will entail no loss of accuracy.

We insert Eq. (2.6) into Eq. (3.1) and recognize that the t' averaging suppresses terms oscillating at optical frequencies, leaving

$$\psi(\tau,r,t)=\frac{1}{T}\int_{t-T/2}^{t+T/2}dt'E(r,t'+\tau)E(r,t')^*+\text{c.c.} \tag{3.2}$$

Then, using the solution (2.30),

$$\begin{aligned}\psi(\tau,r,t)=&\frac{1}{T}\int_{t-T/2}^{t+T/2}dt'\int d^3r_1d^3r_2\int_{-\infty}^{t'+\tau}dt_1\int_{-\infty}^{t'}dt_2\\&\times G(r,t'+\tau;r_1,t_1)G(r,t';r_2,t_2)^*\\&\times F(r_1,t_1)F(r_2,t_2)^*+\text{c.c.}\end{aligned} \tag{3.3}$$

When the ensemble average is taken to get $\langle\psi(\tau,r,t)\rangle$, it is the nonvanishing average $\langle F(r_1,t_1)F(r_2,t_2)^*\rangle$ that results. We anticipate that source correlations will be short ranged in both space and time [24], and are tempted to write

$$\langle F(r_1,t_1)F(r_2,t_2)^*\rangle=D_{\text{FF}}(r_1,t_1)\,\delta(t_1-t_2)\,\delta(r_1-r_2).$$

However, the *actual* time range of the correlated average is on the order of $\tau_{\text{pol}}\approx10^{-13}$ seconds. Although this is short on the time scale over which functions like E_ν and $g_{\mu\nu}$ vary, it is long on the time scale on which the phase factors in Eq. (2.20) vary. For this reason, we cannot yet go to a $\delta(t_1-t_2)$ time correlation function. Instead, we write

$$\begin{aligned}&\langle F(r_1,t_1)F(r_2,t_2)^*\rangle\\&\quad=\delta(r_1-r_2)\int_{-\infty}^{\infty}d\omega\,2D_\omega(r_1,\overline{t})e^{i\omega(t_2-t_1)},\end{aligned} \tag{3.4}$$

where $\overline{t}=(t_1+t_2)/2$. We insert Eqs. (3.4) and (2.21) into the ensemble average of Eq. (3.3) to get

$$\langle\psi(\tau,r,t)\rangle=\frac{1}{T}\int_{t-T/2}^{t+T/2}dt'\sum_{\mu\nu}\sum_{\mu'\nu'}\hat{E}_\mu(r,t'+\tau)\hat{E}_{\mu'}(r,t')^*\times\int_{-\infty}^{\infty}d\omega\int_{-\infty}^{t'+\tau}dt_1\int_{-\infty}^{t'}dt_2\times g_{\mu\nu}(t'+\tau,t_1)f_\nu^\omega(t_1)g_{\mu'\nu'}(t',t_2)^*f_{\nu'}^\omega(t_2)^*\times I_{\nu\nu'}^\omega(t_1,t_2)+\text{c.c.},\tag{3.5}$$

where

$$f_\nu^\omega(t)\equiv\exp i\int_0^t[\omega_\nu(s)-\omega]ds\tag{3.6a}$$

and

$$I_{\nu\nu'}^\omega(t_1,t_2)\equiv\int d^3r_1E_\nu(r_1,t_1)2D_\omega(r_1,\overline{t})E_{\nu'}(r_1,t_2)^*.\tag{3.6b}$$

In the t_1 integration, $f_\nu^\omega(t_1)$ is a phase factor that oscillates with a frequency $\omega-\omega_\nu(t_1)$. If this oscillation is rapid, this part of the t_1 integrand will not contribute to the integral. The contribution to the t_1 integral comes only from those regions of t_1 for which $\omega_\nu(t_1)\approx\omega$. Similarly, contributions to the t_2 integral come only where $\omega_{\nu'}(t_2)\approx\omega$. Taking these considerations together, the contribution to the t_1t_2 integral comes from those regions in the t_1t_2 plane for which

$$\omega_\nu(t_1)\approx\omega\approx\omega_{\nu'}(t_2).$$

$|t_1-t_2|$ is constrained to be less than τ_{pol}. $\omega_{\nu'}(t_2)$ can undergo only very small changes during this time period, and so the above could have been written

$$\omega_\nu(t_1)\approx\omega\approx\omega_{\nu'}(t_1).$$

The only way to satisfy $\omega_\nu(t_1)=\omega_{\nu'}(t_1)$ is to have $\nu'=\nu$. We therefore drop all $\nu\neq\nu'$ terms in Eq. (3.5) to get

$$\langle\psi(\tau,r,t)\rangle=\frac{1}{T}\int_{t-T/2}^{t+T/2}dt'\sum_{\mu\mu'\nu}\hat{E}_\mu(r,t'+\tau)\hat{E}_{\mu'}(r,t')^*\times\int_{-\infty}^{\infty}d\omega\int_{-\infty}^{t'+\tau}dt_1\int_{-\infty}^{t'}dt_2\times g_{\mu\nu}(t'+\tau,t_1)g_{\mu'\nu}(t',t_2)^*I_{\nu\nu}^\omega(t_1,t_2)\times\exp i\int_{t_2}^{t_1}[\omega_\nu(s)-\omega]ds+\text{c.c.}\tag{3.7}$$

The ω integration can be carried out. We make use of the small change in $\omega_\nu(s)$ over the time span in the s integral to approximate

$$\int_{-\infty}^{\infty}d\omega\,2D_\omega(r_1,\overline{t})e^{i\int_{t_2}^{t_1}[\omega_\nu(s)-\omega]ds}=\int_{-\infty}^{\infty}d\omega\,2D_\omega(r_1,\overline{t})e^{i[\omega_\nu(t_1)-\omega](t-t_2)}=2\pi\delta(t_1-t_2)2D_\nu(r_1,t_1),\tag{3.8}$$

where D_ν means D_ω evaluated at $\omega=\omega_\nu(t_1)$. The $\delta(t_1-t_2)$ is justified here because there are no longer any rapidly varying terms in the integrand. Using this to carry out the t_2 integration,

$$\langle\psi(\tau,r,t)\rangle=\frac{1}{T}\int_{T-\tau/2}^{T+\tau/2}dt'\sum_{\mu\mu'\nu}\hat{E}_\mu(r,t'+\tau)\hat{E}_{\mu'}(r,t')^*\times\int_{-\infty}^{t'}dt_1g_{\mu\nu}(t'+\tau,t_1)g_{\mu'\nu}(t't_1)^*\times\int d^3r_1I_\nu(t_1)+\text{c.c.},\tag{3.9a}$$

where

$$I_\nu(t_1)\equiv2\pi\int d^3r_12D_\nu(r_1,t_1)|E_\nu(r_1,t_1)|^2.\tag{3.9b}$$

It will turn out later that D_ν is real, so that I_ν is too.

The power spectrum $P(\omega,r,t)$ can be obtained from the correlation function $\langle\psi(\tau,r,t)\rangle$ by the Wiener-Khinchine theorem: the two are ω-τ Fourier transforms of each other [23]:

$$P(\omega,r,t)=\frac{1}{2\pi}\int d\tau\langle\psi(\tau,r,t)\rangle e^{-i\omega\tau}.\tag{3.10}$$

If we are interested in the short-term power spectrum (such as would be measured by a spectrometer with very fast time resolution), we can discard the T averaging and replace the function being averaged over by its value at $t'=t$. In this case, Eq. (3.9) becomes

$$\langle\psi(\tau,r,t)\rangle=\sum_{\mu\mu'\nu}\hat{E}_\mu(r,t+\tau)\hat{E}_{\mu'}(r,t)^*\times\int_{-\infty}^{t}dt_1g_{\mu\nu}(t+\tau,t_1)g_{\mu'\nu}(t,t_1)^*I_\nu(t_1)+\text{c.c.}\tag{3.11}$$

Because we are not concerned with line breadth here (e.g., phase-fluctuation-induced spectral broadening or finite photon residence time in the cavity), the Fourier transform (3.10) can be bypassed in the following way. The total power is given by evaluating Eq. (3.11) at $\tau=0$,

$$P(r,t)=\tfrac{1}{2}\sum_{\mu\mu'}\hat{E}_\mu(r,t)\hat{E}_{\mu'}(r,t)^*S_{\mu\mu'}(t)+\text{c.c.},\tag{3.12a}$$

where

$$S_{\mu\mu'}(t) \equiv \sum_{\nu} \int_{-\infty}^{t} dt_1 g_{\mu\nu}(t,t_1) g_{\mu'\nu}(r,t)^* R_{\nu}^{\rm sp}(t_1) \tag{3.12b}$$

and

$$R_{\nu}^{\rm sp}(t_1) \equiv 2 I_{\nu}(t_1). \tag{3.12c}$$

We refer to $S_{\mu\mu'}(t)$ as the photon number matrix because, as we shall see below, its diagonal elements have the significance of being proportional to the number of photons in the μth mode.

There are two spectra that might be of interest. The first arises from the periodic modulation of the laser. To obtain it, one must evaluate the averaged correlation function (3.9) with T being the complete modulation period, and then take the Fourier transform (3.10). The second is what would be observed in a spectrometer fast enough to follow the frequency chirp associated with any transients but not fast enough to observe beating (if any) between a pair of simultaneously lasing modes. In that case, the time T used for the averaging in Eq. (3.9a) should be taken large enough that $\Delta\omega T \gg 2\pi$. The t' dependence of $\tilde{E}_{\mu}\tilde{E}^*_{\mu'}$ averages the term away unless $\mu = \mu'$. This results in a diagonal photon number matrix, and the power in the μth mode becomes

$$P_{\mu}(r,t) = |E_{\mu}(r,t)|^2 S_{\mu\mu}(t) \tag{3.13a}$$

where

$$S_{\mu\mu}(t) \equiv \sum_{\nu} \int_{-\infty}^{t} dt_1 |g_{\mu\nu}(t,t_1)|^2 R_{\nu}^{\rm sp}(t_1). \tag{3.13b}$$

When the photon number matrix is diagonal (and only then), the frequency associated with the μth mode is given by writing that term in Eq. (3.11) in phasor notation and taking the τ derivative of its total phase at $\tau = 0$. That is, we write

$$E_{\mu}(r,t+\tau) = R_{\mu}(r,t+\tau) e^{-i\phi_{\mu}(r,t+\tau)} \tag{3.14a}$$

with R_{μ} and ϕ_{μ} both real. Then the frequency is

$$\omega_{\mu}(r,t) = \omega_{\mu}(t) + \frac{d}{dt}\phi_{\mu}(r,t). \tag{3.14b}$$

Although one might have expected a contribution from the τ-dependent phase of $g_{\mu\nu}(t+\tau,t_1)$, we show in Appendix B that the anticipated contribution vanishes and that Eq. (3.14) is correct as written. It is the form of Eq. (3.13) that gives the diagonal elements of $S_{\mu\mu'}(t)$ the significance of being photon numbers, although for them to actually equal the number of photons in the cavity, a different normalization is needed.

We now derive the rate equation satisfied by the diagonal elements of the photon number matrix, the ''photon numbers.'' Differentiating $S_{\mu\mu}$ with respect to t gives

$$\frac{d}{dt} S_{\mu\mu}(t) \equiv \int_{-\infty}^{t} dt_1 \sum_{\nu} \frac{\partial}{\partial t} |g_{\mu\nu}(t,t_1)|^2 R_{\nu}^{\rm sp}(t_1) + \sum_{\nu} |g_{\mu\nu}(t,t)|^2 R_{\nu}^{\rm sp}(t). \tag{3.15}$$

Note that, from the fact that λ_{μ} is pure imaginary,

$$\frac{\partial}{\partial t} |g_{\mu\nu}(t,t')|^2 = 2i\lambda_{\mu}(t) |g_{\mu\nu}(t,t')|^2 - 2\,\mathrm{Re} \sum_{\kappa \neq \mu} g_{\mu\nu}(t,t')^* T_{\mu\kappa}(t) g_{\kappa\nu}(t,t'), \tag{3.16}$$

while, from Eq. (2.29),

$$g_{\mu\nu}(t,t) = \delta_{\mu\nu}. \tag{3.17}$$

This reduces Eq. (3.15) to

$$\frac{dS_{\mu\mu}}{dt} = 2i\lambda_{\mu}(t) S_{\mu\mu}(t) + R_{\mu}^{\rm sp}(t) + \Xi_{\mu}(t), \tag{3.18}$$

where $\Xi_{\mu}(t)$ is defined by the integral

$$\Xi_{\mu}(t) = \sum_{\nu} \int_{-\infty}^{t} dt_1 R_{\nu}^{\rm sp}(t_1) \mathcal{T}(\nu,t_1 \to \mu,t) \tag{3.19}$$

and

$$\mathcal{T}(\nu,t_1 \to \mu,t) \equiv -2\,\mathrm{Re} \sum_{\kappa \neq \mu} T_{\mu\kappa}(t) g_{\mu\nu}(t,t_1)^* g_{\kappa\nu}(t,t_1). \tag{3.20}$$

In the adiabatic approximation, $\mathcal{T}$ oscillates so rapidly that $\Xi_{\mu}(t)$ will vanish. Comparing Eq. (3.18) to Eq. (1.2) in that case demands that we make the identification

$$2i\lambda_{\mu}(t) = G_{\mu}(t) - \frac{1}{\tau_{\mu}(t)}, \tag{3.21}$$

so that Eq. (3.18) is

$$\frac{dS_{\mu\mu}}{dt} = \left(G_{\mu} - \frac{1}{\tau_{\mu}} \right) S_{\mu\mu} + R_{\mu}^{\rm sp} + \Xi_{\mu}. \tag{3.22}$$

This is the equation that replaces the standard rate equation (1.1) when the adiabatic approximation starts to break down. It differs from it in only a single term. From the form of Eqs. (3.19) and (3.22), we infer that $\Xi_{\mu}(t)$, the additional term, is proportional to the rate at which photons emitted into other modes ν at earlier times t_1 and amplified since are now being supplied to the μth mode. As a consequence of the enhanced supply of photons to the side modes, the side-mode amplitude will be larger than it would be without this additional source. Thus, one effect of the breakdown of the adiabatic approximation is to decrease the side-mode suppression ratio.

Using Eq. (3.22) as a numerical method to update the photon number is exceedingly cumbersome because of Eq.

(3.19), an integral over past time. However, in Sec. V, we shall present a simple and efficient numerical way to update $S_\mu(t)$ with not much more effort than is used to solve Eq. (3.22) in the absence of Ξ_μ.

IV. SPONTANEOUS-EMISSION TERM

In the equilibrium time-independent system, the rate of spontaneous emission depends on the (imaginary part of) the dielectric constant of the medium and on the amount of population inversion [2,25,26]. If these are time dependent, the rate might be an integral over their present and past values or might depend on other dynamic considerations. We are unaware of any theory relevant to this point and will assume instead that the emission rate at time *t* depends on the dielectric constant and inversion only at time *t*. The diffusion constant needed here has been derived by Henry ([2], Eqs. 38 and 45) and it is real:

$$2D_\omega(r,t)=\frac{4\omega^4\hbar\varepsilon''_\omega(r,t)}{c^4}\langle n_\omega(r,t)\rangle, \tag{4.1a}$$

$$\langle n_\omega(r,t)\rangle\equiv[e^{[\hbar\omega-eV(r,t)]/kT}-]^{-1}, \tag{4.1b}$$

where $\varepsilon''_\omega(r,t)$ is the imaginary part of the dielectric constant and $V(r,t)$ is the separation between the electron and hole quasi-Fermi-energies.

V. AN EFFICIENT NUMERICAL ALGORITHM FOR EVALUATING $S_{\mu\mu'}(t)$

The rate equations (3.18)–(3.20) contain a term $\Xi_\nu(t)$ which counts photons that were emitted into other modes at an earlier time, amplified there, and are now leaking into the νth mode. The evaluation of $\Xi_\nu(t)$ involves an integral over the entire past history of the laser, which may be computationally prohibitive. In this section, we provide an efficient and accurate algorithm for stepping the laser forward in time without having to retain any history prior to the start of the current time step.

Using Eq. (2.20), the Green's function (2.31) can be written as

$$G(r,t;,r_1,t_1)=\frac{1}{i}\sum_{\mu\nu} E_\mu(r,t)G_{\mu\nu}(t,t_1)E_\nu(r_1,t_1), \tag{5.1}$$

where

$$G_{\mu\nu}(t,t')\equiv e^{-i\int_0^t\omega_\mu(\tau)d\tau}g_{\mu\nu}(t,t')e^{i\int_0^t\omega_\nu(\tau)d\tau}. \tag{5.2}$$

Because of Eq. (2.29), the elements $G_{\mu\nu}$ satisfy

$$[(\lambda_\mu(t)-\omega_\mu(t)]G_{\mu\nu}(t,t')+i\frac{\partial}{\partial t}G_{\mu\nu}(t,t')$$

$$+i\sum_{\kappa\neq\mu} t_{\mu\kappa}(t)G_{\kappa\nu}(t,t')=0, \tag{5.3a}$$

$$G_{\mu\nu}(t',t')=\delta_{\mu\nu}. \tag{5.3b}$$

We define the matrix $M_{\mu\nu}(t)$ by

$$M_{\mu\nu}(t)\equiv-i\tilde{\omega}_\mu(t)\delta_{\mu\nu}-t_{\mu\nu}(t) \tag{5.4}$$

where $\tilde{\omega}_\mu$ and $t_{\mu\nu}$ are defined in Eqs. (2.26) and (2.27). $G_{\mu\nu}(t,t')$ then satisfies the matrix differential equation and boundary condition

$$\frac{\partial}{\partial t}G(t,t')=M(t)G(t,t'), \tag{5.5a}$$

$$G(t',t')=I. \tag{5.5b}$$

G and *M* are $m\times m$ matrices, *m* being the number of coupled modes, and *I* is the identity matrix. The solution to Eq. (5.5) is

$$G(t,t')=\mathcal{T}\left(\exp\int_{t'}^{t}M(\tau)d\tau\right) \tag{5.6}$$

where $\mathcal{T}$ is the usual time-ordering operator [27], ordering later times to the left. From this solution, it follows that for $t_1\leqslant t_2\leqslant t_3$,

$$G(t_3,t_1)=G(t_3,t_2)G(t_2,t_1). \tag{5.7}$$

We take $\Delta t>0$ and use this property in the form

$$G(t+\Delta t,t')=g(t+\Delta t,t)G(t,t'), \tag{5.8}$$

where

$$g(t+\Delta t,t)\equiv\mathcal{T}\left(\exp\int_{t}^{t+\Delta t}M(\tau)d\tau\right). \tag{5.9}$$

In Appendix C, we show that the time-ordered exponential (5.9) can be written as an ordinary exponential with a correction term:

$$\mathcal{T}\left(\exp\int_{t}^{t+\Delta t}M(\tau)d\tau\right)=\left(\exp\int_{t}^{t+\Delta t}M(\tau)d\tau\right)+E(t,\Delta t). \tag{5.10}$$

The lowest-order term in the series for $E(t,\Delta t)$ is given by an integral over a two-time commutator of $M(\tau)$:

$$E_2(t,\Delta t)=\frac{1}{2!}\int_t^{t+\Delta t}d\tau_1\int_t^{\tau_1}d\tau_2[M(\tau_1),M(\tau_2)].$$

To estimate the size of the error term, we expand $M(\tau)$ to first order about $\tau=t$ so that

$$[M(\tau_1),M(\tau_2)]\approx(\tau_1-\tau_2)[\dot{M}(t),M(t)].$$

This gives the following error estimate and criterion:

$$E_2(t,\Delta t)\approx\frac{(\Delta t)^3}{12}[\dot{M}(t),M(t)]\ll 1. \tag{5.11}$$

To evaluate the exponential, we write

$$\int_t^{t+\Delta t} M(\tau)d\tau \approx \tfrac{1}{2}\,\Delta t[M(t+\Delta t)+M(t)] - \tfrac{1}{12}\,(\Delta t)^3 \ddot{M}. \tag{5.12}$$

The second term, which will be dropped, is regarded as a correction to the first and so the condition for acceptable accuracy is

$$\tfrac{1}{12}\,\ddot{M}(t)(\Delta t)^2 \ll M(t). \tag{5.13}$$

When both conditions (5.11) and (5.13) are satisfied, the exponential operator can be evaluated by diagonalizing,

$$Q^{-1}\tfrac{1}{2}\,[M(t+\Delta t)+M(t)]Q = D, \tag{5.14}$$

where D is diagonal. The matrix exponential is then

$$\exp\left(\frac{\Delta t}{2}[M(t+\Delta t)+M(t)]\right) = Q\,\exp(D\,\Delta t)Q^{-1}. \tag{5.15}$$

This is the working formula for evaluating $g(t+\Delta t,t)$.

Finally, to update the photon number, we regard Eq. (3.12b), the photon number matrix $S_{\mu\nu}(t+\Delta t)$, as the $\mu\nu$ element of

$$S(t+\Delta t) = \int_{-\infty}^{t+\Delta t} dt'\,G(t+\Delta t,t')R(t')G^H(t+\Delta t,t'). \tag{5.16}$$

$R(t')$ is diagonal and the superscript H denotes the Hermitian conjugate matrix. We break the integral into

$$S(t+\Delta t) = \int_{-\infty}^{t} dt'\,G(t+\Delta,t')R(t')G^H(t+\Delta t,t') + \int_{t}^{t+\Delta t} dt'\,G(t+\Delta t,t')R(t')G^H(t+\Delta t,t'). \tag{5.17}$$

Then using Eqs. (5.5b) and (5.8),

$$S(t+\Delta t) = g(t+\Delta t,t)S(t)g^H(t+\Delta t,t) + \int_{t}^{t+\Delta t} dt'\,g(t+\Delta t,t')R(t')g^H(t+\Delta t,t'), \tag{5.18a}$$

where

$$g(t+\Delta t,t') = Q\,\exp[(t+\Delta t-t')D]Q^{-1}. \tag{5.18b}$$

This is the recursive algorithm for evaluating $S(t+\Delta t)$ using knowledge of $S(t)$ at the previous time step and of $R(t')$ over the interval $t<t'<t+\Delta t$. The recursive algorithm (5.18) is started at time t_0, prior to which the laser has been in a steady state, so that

$$S_{\mu\nu}(t_0) = \frac{R_\nu^{\rm sp}(t_0)}{1/\tau_\nu(t_0) - G_\nu(t_0)}\,\delta_{\mu\nu}. \tag{5.19}$$

When the time dependence of the laser is slow, the criteria (5.11) and (5.13) allow for much larger time steps, and the algorithm will automatically step forward rapidly, slowing down only when rapid time dependence of the laser demands shorter time steps.

VI. SUMMARY

In this paper, we have studied the conditions under which the usual multimode semiconductor laser rate equations are valid and have found a criterion for their validity. We derived a new rate equation to be used when the usual one is invalid, and have given a constructive algorithm for numerically solving it. Our analysis applies to all situations in which the laser field is expanded in ''adiabatic'' modes, that is, eigenmodes of some time-dependent equation in which the dielectric constant is regarded as being parametrically dependent on the time. We showed that when a linear combination of such modes is used to solve the time-dependent wave equation, there do arise nonadiabatic couplings between these adiabatic modes. We showed that the resulting rate equation, including the nonadiabatic couplings, takes the form of coupled-mode rate equations in which the usual spontaneous emission term is augmented by a term $\Xi_\mu(t)$. $\Xi_\mu(t)$ counts photons that were emitted spontaneously at earlier times into other modes and which are now, due to the breakdown of the adiabatic approximation, leaking into the mode of interest, providing an additional source of photons. The additional source takes the form of an integral over all earlier times. This is inconvenient computationally, and so we provided an algorithm to advance the photon number using only information that refers to the present time step. The algorithm allows the new equation to be solved with substantially the same effort as the usual one, and provides, moreover, error estimates at each step of the way.

The validity of the adiabatic approximation, and hence of the *ordinary* rate equations, was shown to depend on the product of two dimensionless factors, essentially $\nu_{\max}T_p$ and $\langle\Delta\varepsilon/\varepsilon\rangle$, being less than $(1/\nu_0T_p)(1-\nu_{\max}T_p)$. $\nu_{\max}$ is the maximum frequency of modulating the laser, ν_0 is the optical frequency, T_p is the photon round-trip time in the laser cavity, and $\langle\Delta\varepsilon/\varepsilon\rangle$ is the spatial average of the largest fractional change in dielectric constant during the modulation. Thus, there is no problem with the usual rate equation at low modulation rates, nor in the small-signal regime where the change in dielectric constant is order small, nor in the short-optical-axis regime, such as in vertical cavity surface emitting lasers. However, as the need for modeling moves out of these regimes, it will become necessary to take $\Xi_\mu(t)$, or something equivalent to it, into account.

Finally, lest it be thought that $\Xi_\nu(t)$ and the whole idea of the breakdown of the adiabatic approximation is an artifact of our use of the eigenmode expansion for the electric field rather than the usual traveling-wave equations, we should point out that traveling-wave equations are derived assuming that the dielectric constant $\varepsilon_\omega(r)$ is independent of time. When the equations are rederived allowing for a time-dependent dielectric function, an explicit $\partial\varepsilon_\omega/\partial t$ appears in them too. Although we have not studied the conditions under which $\partial\varepsilon_\omega/\partial t$ can be ignored in the traveling-wave equations, there is no reason to believe that the conditions are any different from those that allow us, in this paper, to ignore $\Xi_\nu(t)$.

APPENDIX A: CRITERION FOR USE OF THE ADIABATIC APPROXIMATION

The adiabatic approximation is that off-diagonal elements $g_{\mu\nu}(t,t')$ do not build up from their initial value of zero. As a result, the diagonal elements are given by Eq. (2.32a). To establish a condition for validity of this approximation, evaluate $g_{\mu\nu}$ for $\mu\neq\nu$ to first order in $T_{\mu\nu}(t)$. We integrate Eq. (2.29a) from t' to T, using the zeroth-order approximation (2.32a) in the expression for $\partial g_{\mu\nu}/\partial t$. The result is

$$g_{\mu\nu}(T,t')=-\int_{t'}^{T}dt\,T_{\mu\nu}(t)e^{i\int_0^{t}\lambda_\nu(\tau)d\tau}. \tag{A1}$$

For size estimation, we regard λ_ν, ω_μ, and ω_ν in Eq. (2.22b) as being independent of τ. Further, we take

$$t_{\mu\nu}(t)=t_{\mu\nu}e^{-i\omega_{\max}t} \tag{A2}$$

where $\omega_{\max}$ is the maximum modulation frequency. The expression (A1) then becomes

$$g_{\mu\nu}(T,t')=\frac{it_{\mu\nu}}{\omega_\mu-\tilde{\omega}_\nu-\omega_{\max}}\times[e^{i(\omega_\mu-\omega_\nu-\omega_{\max})T}e^{i\lambda_\nu(T-t')}-e^{i(\omega_\mu-\omega_\nu-\omega_{\max})t'}]. \tag{A3}$$

Since $\mathrm{Im}\,\lambda_\nu>0$, each of the exponentials in the large parentheses is at most of order unity, and their difference cannot exceed 2. Putting in the value of $t_{\mu\nu}$ from Eq. (2.27) and neglecting the small imaginary part of $\tilde{\omega}$ in the denominator, we have

$$g_{\mu\nu}(T,t')\approx\frac{2(\omega_\nu/c)^2\langle E_\mu|\dot{\varepsilon}_\nu|E_\nu\rangle}{(\omega_\mu-\omega_\nu)(\omega_\mu-\omega_\nu-\omega_{\max})}. \tag{A4}$$

This can be put in a form independent of the normalization of the wave functions by dividing by the normalization (2.19b):

$$g_{\mu\nu}(T,t')\approx\frac{2(\omega_\nu/c)^2\langle E_\mu(\dot{\varepsilon}_\nu)E_\nu\rangle}{\langle E_\nu K_\nu^2 E_\nu\rangle}\,\frac{1}{(\omega_\mu-\omega_\nu)(\omega_\mu-\omega_\nu-\omega_{\max})}. \tag{A5}$$

The first factor can also be written as

$$\frac{\omega_\nu\langle E_\mu|\dot{\varepsilon}_\nu|E_\nu\rangle}{\langle E_\nu|\varepsilon_\nu+(\omega_\nu/2)(\partial\varepsilon_\nu/\partial\omega)|E_\nu\rangle}.$$

The largest value of the second factor is when $\nu=\mu-1$, and then $\omega_\mu-\omega_{\mu+1}\approx 2\pi/T_p$. In such case, the condition that $g_{\mu\nu}\ll 1$ is

$$\frac{\langle E_\mu|\varepsilon_d|E_\nu\rangle}{\langle E_\nu|\varepsilon_\nu+(\omega_\nu/2)(\partial\varepsilon_\nu/\partial\omega)|E_\nu\rangle}\,\omega_{\max}T_p\ll\frac{(2\pi)^2}{\omega_\nu T_p}\left(1-\frac{\omega_{\max}T_p}{2\pi}\right), \tag{A6}$$

where we have taken $\dot{\varepsilon}_\nu\approx\omega_{\max}\varepsilon_d$, with ε_d being the dynamic part of the dielectric function at frequency ω_ν.

APPENDIX B: THE FREQUENCY ASSOCIATED WITH $g_{\mu\nu}(t+\tau,t_1)$

We shall now show that Eq. (3.13) contains no frequency attributable to the τ-dependent phase of $g_{\mu\nu}(t+\tau,t_1)$. The frequency under study is the τ derivative of the phase, evaluated in the limit $\tau\to 0$. The proof consists of showing that the phase contains no part that is linear in τ, and thus that the derivative vanishes in this limit. The idea is to express $g_{\mu\nu}$ in terms of the appropriate time-ordered exponential, as was done for $G_{\mu\nu}$ in Sec. V. In this way, analogous to Eq. (5.8), we have

$$g_{\mu\nu}(t+\tau,t_1)=\sum_\kappa\left[\mathcal{T}\exp\int_t^{t+\tau}\tilde{M}(t')dt'\right]_{\mu\kappa}g_{\kappa\nu}(t,t_1), \tag{B1}$$

where $\mathcal{T}$ is the time-ordering operator and the matrix $\tilde{M}(t)$ is defined, using Eq. (2.29), as

$$\tilde{M}_{\mu\kappa}(t)=i\lambda_\mu(t)\delta_{\mu\kappa}-T_{\mu\kappa}(t)(1-\delta_{\mu\kappa}). \tag{B2}$$

Working to lowest order in τ,

$$\left[\mathcal{T}\exp\int_t^{t+\tau}M(t')dt'\right]_{\mu\kappa}=[1+\tau\tilde{M}(t)]_{\mu\kappa}=[1+i\tau\lambda_\mu(t)]\delta_{\mu\kappa}-\tau T_{\mu\kappa}(t)(1-\delta_{\mu\kappa}). \tag{B3}$$

The diagonal element is purely real because $\lambda_\mu(t)$ is pure imaginary, so its phase is zero. The complex off-diagonal elements have a ratio of real to imaginary part that does not depend on τ, so their phase is also τ independent.

APPENDIX C: THE ERROR ESTIMATE $E(t,\Delta t)$

The error estimate in Eq. (5.10) is

$$E(t,\Delta t)\equiv\mathcal{T}\left(\exp\int_t^{t+\Delta t}M(\tau)d\tau\right)-\left(\exp\int_t^{t+\Delta t}M(\tau)d\tau\right), \tag{C1}$$

where $\mathcal{T}$ is the time-ordering operator, ordering later times to the left. For simplicity, we put $t=0$. The exponential and the time-ordered exponential are both expanded as power series:

$$\mathcal{T}\left(\exp\int_0^{\Delta t}M(\tau)d\tau\right)=\sum_{n=0}\frac{1}{n!}\int_0^{\Delta t}d\tau_1\int_0^{\Delta t}d\tau_2\cdots\int_0^{\Delta t}d\tau_n \times\mathcal{T}M(\tau_1)M(\tau_2)\cdots M(\tau_n),$$

$$\left(\exp\int_0^{\Delta t}M(\tau)d\tau\right)=\sum_{n=0}\frac{1}{n!}\int_0^{\Delta t}d\tau_1\int_0^{\Delta t}d\tau_2\cdots\int_0^{\Delta t}d\tau_n \times M(\tau_1)M(t_2)\cdots M(\tau_n).$$

As an example of how the terms will be manipulated, consider the third-order term. It contains an integral over a cube of side Δt in τ_1,τ_2,τ_3 space. This cube can be divided into 3! parts, depending on the relative sizes of τ_1, τ_2, and τ_3. Each part is a separate integral. We rearrange the dummy variables τ_1,τ_2,τ_3 so that they stand in ''standard'' order $\tau_3<\tau_2<\tau_1$. Each of the six integrals now has the same limits, but the three matrices $M(\tau_1)$, $M(\tau_2)$, and $M(\tau_3)$ appear in an order dictated by the permutation needed to put the dummy indices in standard order. Each of the 3! permutations appears once. The error term now is given as the series

$$E(\Delta t,0)=\sum_{n=0}\frac{1}{n!}\int_0^{\Delta t}d\tau_1\int_0^{\tau_1}d\tau_2\cdots\int_0^{\tau_{n-1}}d\tau_n \times(\mathcal{T}-1)\sum P_N M(\tau_1)M(\tau_2)\cdots M(\tau_n). \tag{C2}$$

The inner sum is over all possible permutations of the τ_j indices. In Eq. (C2) the time-ordering operator $\mathcal{T}$ rearranges the matrices following it so that, no matter in what order they are written, matrices evaluated at earlier times stand to the right of those evaluated at later times. As a result, each of the order-permuted matrices following $\mathcal{T}$ is returned to ''standard'' order $M(\tau_1)M(\tau_2)\cdots M(\tau_n)$. The second-order term, the first nonzero one, is

$$M(\tau_1)M(\tau_2)+M(\tau_1)M(\tau_2)-M(\tau_1)M(\tau_2)-M(\tau_2)M(\tau_1) =[M(\tau_1),M(\tau_2)]. \tag{C3}$$

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