Efficient analytic computation of dispersion from multilayer structures

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We demonstrate an inductive method for computing exact derivatives of reflection phase for layered media using the transfer matrix formalism. The algorithm scales linearly with the number of layers. We show a physically realistic approximation that leads to an efficient procedure for accurately computing dispersion significantly faster than with standard finite difference methods. We discuss the theory behind the approximation and show results for a dispersion compensating chirped mirror from a Ti:Sa laser.

OCIS codes: 310.6860, 310.0310, 320.0320.

1. Introduction

The design and fabrication of dispersive optical thin-film filters and mirrors is very important for the generation of few-cycle laser pulses approaching the single-cycle regime.[1–4] Efficient and accurate calculation of dispersive properties is crucial for the design and optimization of these multilayer dielectric optical coatings. The standard method for computing the group delay dispersion is to compute complex reflection coefficients using the transfer matrix technique and then take successive finite differences of phase over frequency. For paired mirror systems containing up to 160 layers[4] this leads to a tremendous numerical effort during optimization.

Accurately computing the mth order dispersion at a given wavelength using finite differences (FDs) requires computing at least $(m+1)$ reflection coefficients and taking m differences. Unfortunately, numerical differentiation is inherently unstable[5] and achieving high accuracy requires careful optimization of sample spacing to balance the competing effects of round-off error and truncation error. This issue is especially pertinent in the computation of higher-order dispersion, as is often needed in the analysis of telecommunications filters.

We demonstrate a method to analytically compute dispersion to any order that is $O[n]$ in both storage and execution time,[6] where n is the number of layers. We show how simplifying approximations in the derivative lead to highly efficient algorithms for dispersion calculations. In this regime, the first m derivatives of phase at a given wavelength can be computed in less time than

for m zeroth-order reflection coefficients, resulting in significantly faster computation time than with numerical differentiation and yet without the associated issues of numerical stability.

The methods discussed here are useful in optimization algorithms where single values of dispersion (as opposed to gradients of the dispersion) are needed, such as in line search algorithms or stochastic optimizations. They are also useful for the accurate evaluation of dispersion around resonances where accurate numerical differentiation is problematic. In a follow-up paper, we will extend these methods to the $O[n]$ computation of analytic dispersion gradients for the refinement of multilayer structures.

2. Analytic Computation of Phase Derivatives

In the foregoing we will consider a lossless dielectric stack whose total transfer matrix[7] is given by

$$\mathbf{T}_{(n,0)} = \begin{pmatrix} a(\omega) & b(\omega) \\ b^*(\omega) & a^*(\omega) \end{pmatrix} \equiv \begin{pmatrix} |a(\omega)|\, e^{j\phi_a(\omega)} & |b(\omega)|\, e^{j\phi_b(\omega)} \\ |b(\omega)|\, e^{-j\phi_b(\omega)} & |a(\omega)|\, e^{-j\phi_a(\omega)} \end{pmatrix}. \tag{1}$$

In our notation, illustrated in Figure 1, $\mathbf{T}_\ell$ will refer to the transfer matrix of the ℓth layer, which includes the interface between it and the previous medium and propagation through the layer up to, but not across, the next interface. (The substrate can be handled as a final zero-thickness layer in this scheme.) Furthermore, we'll let $\mathbf{T}_{(\ell_2,\ell_1)} \equiv \mathbf{T}_{\ell_2} \cdots \mathbf{T}_{\ell_1+2}\mathbf{T}_{\ell_1+1}$ refer to the matrix that goes from the end of layer ℓ_1 to the end of layer ℓ_2, including all interfaces in between those layers. By convention, our transfer matrices operate on a vector space where the first and second elements represent forward and reverse propagating fields. The complex reflection coefficient Γ at the input to the first layer is thus given by

$$\Gamma(\omega) \equiv |\Gamma(\omega)|\, e^{j\phi(\omega)} = -\frac{b^*(\omega)}{a^*(\omega)}. \tag{2}$$

The reflection phase is then

$$\phi(\omega) = \phi_a(\omega) - \phi_b(\omega) + \pi, \tag{3}$$

and so the kth order dispersion is simply

$$\phi^{(k)}(\omega) = \phi_a^{(k)}(\omega) - \phi_b^{(k)}(\omega). \tag{4}$$

2.A. Inductive computation of transfer matrix derivatives

The mth order dispersion for reflection from the structure is a function of the first m complex derivatives of $\mathbf{T}_{(n,0)}$ (see Section 2.B). Since $\mathbf{T}_{(n,0)}$ can be computed analytically for a given wavelength, in theory we should be able to find any derivative analytically. To avoid a combinatorial explosion of terms, however, we must do so inductively. We calculate $\mathbf{T}_{(\ell,0)}$ and its derivatives from the $(m+1)$ derivatives (zeroth through mth order) of the matrix for the ℓth layer, $\mathbf{T}_\ell$, and of

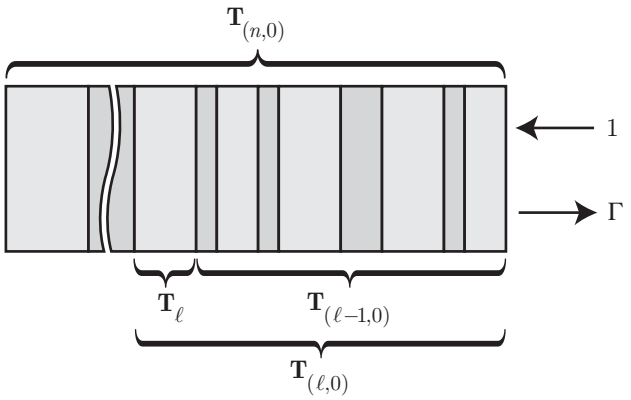

Fig. 1. Diagram showing transfer matrix notation.

the cumulative transfer matrix for the preceding layers, $\mathbf{T}_{(\ell-1,0)}$. This is done by simply evaluating terms of the following form:

$$\frac{\partial^k \mathbf{T}_{(\ell,0)}}{\partial \omega^k} = \frac{\partial^k \left(\mathbf{T}_\ell \mathbf{T}_{(\ell-1,0)}\right)}{\partial \omega^k}. \tag{5}$$

As we trace through the stack layer-by-layer, we only need to keep track of $(m+1)$ matrices as we go along.

To calculate the recurrence relation for the kth derivative of the transfer matrix from the beginning of the structure up to the ℓth layer, we simply apply matrix derivative product rules to (5). The induction rules for the first three derivatives , enough to compute third order dispersion (TOD), are

$$\mathbf{T}_{(\ell,0)} = \mathbf{T}_\ell \mathbf{T}_{(\ell-1,0)}, \tag{6}$$

$$\frac{\partial \mathbf{T}_{(\ell,0)}}{\partial \omega} = \frac{\partial \mathbf{T}_\ell}{\partial \omega}\mathbf{T}_{(\ell-1,0)} + \mathbf{T}_\ell \frac{\partial \mathbf{T}_{(\ell-1,0)}}{\partial \omega}, \tag{7}$$

$$\frac{\partial^2 \mathbf{T}_{(\ell,0)}}{\partial \omega^2} = \frac{\partial^2 \mathbf{T}_\ell}{\partial \omega^2}\mathbf{T}_{(\ell-1,0)} + 2\frac{\partial \mathbf{T}_\ell}{\partial \omega}\frac{\partial \mathbf{T}_{(\ell-1,0)}}{\partial \omega} + \mathbf{T}_\ell \frac{\partial^2 \mathbf{T}_{(\ell-1,0)}}{\partial \omega^2}, \tag{8}$$

$$\frac{\partial^3 \mathbf{T}_{(\ell,0)}}{\partial \omega^3} = \frac{\partial^3 \mathbf{T}_\ell}{\partial \omega^3}\mathbf{T}_{(\ell-1,0)} + 3\frac{\partial \mathbf{T}_\ell}{\partial \omega}\frac{\partial^2 \mathbf{T}_{(\ell-1,0)}}{\partial \omega^2} + 3\frac{\partial^2 \mathbf{T}_\ell}{\partial \omega^2}\frac{\partial \mathbf{T}_{(\ell-1,0)}}{\partial \omega} + \mathbf{T}_\ell \frac{\partial^3 \mathbf{T}_{(\ell-1,0)}}{\partial \omega^3}, \tag{9}$$

and so on. Each term on the right hand side above is either known from an induction assumption (i.e. previously computed $\mathbf{T}^{(k)}_{(\ell-1,0)}$ terms) or can be calculated directly (i.e. current layer $\mathbf{T}^{(k)}_\ell$ terms). The only other pieces missing are the trivial statements of the initial matrices:

$$\mathbf{T}_{(0,0)} = \mathbf{I} \quad \text{and} \quad \frac{\partial^k \mathbf{T}_{(0,0)}}{\partial \omega^k} = \mathbf{0}, \quad 0 < k \leq m. \tag{10}$$

Clearly this scheme is still $O[n]$ in the number of layers, as is the standard finite difference method. However, in practice it will be slower. Since each successive derivative requires one more matrix multiplication than its predecessor, the total number of matrix multiplications required

to find the first m derivatives is $O[nm^2]$, whereas finite differences only require $O[nm]$ matrix multiplications. Thus, the fully general case is best used for either low-order dispersion, or when accuracy is more important than speed. In Section 3 we discuss a fast approximate version of this algorithm.

2.B. Computing dispersion from transfer matrix derivatives

The kth phase derivative of $\Gamma(\omega)$ is given by the difference between the kth derivatives of $\phi_a(\omega)$ and $\phi_b(\omega)$, as in (3). However, the derivatives of $\mathbf{T}_{(n,0)}$ which we will calculate with the method of Section 2.A only give us the real and imaginary parts of the derivatives of $a(\omega)$ and $b(\omega)$. We therefore must find the phase (polar coordinate) derivatives in terms of these rectangular terms. There are various ways to do this, most obviously direct computation of the total derivative using coordinate transformations. However, care must be taken to do so in a way that is numerically stable and computationally efficient. Here we briefly illustrate a suitable recursive method and provide explicit solutions for a few initial terms.

Consider the complex function $a(\omega)$ of (1) which can be written as

$$a_r(\omega) + j a_i(\omega) \equiv |a(\omega)|\, e^{j\phi_a(\omega)}. \tag{11}$$

The two terms on the left-hand side, as well as their derivatives, are found in the computation outlined in Section 2.A. A general procedure to find the first m derivatives of $\phi_a(\omega)$ is to take the kth derivative of both sides of (11) and then split the resulting equation into real and imaginary parts to yield two coupled equations. Solving for $\phi_a^{(k)}(\omega)$ and $|a(\omega)|^{(k)}$ then gives solutions in terms of lower polar derivatives and $a_r^{(k)}$ and $a_i^{(k)}$. The lower derivatives can then themselves be solved for in the same manner until everything is finally expressed only in terms of derivatives of $a_r(\omega)$ and $a_i(\omega)$.

The first three derivatives for $\phi_a(\omega)$ found per the above procedure are

$$\phi_a'(\omega) = \frac{1}{|a|}\left[a_i' \cos\phi_a - a_r' \sin\phi_a\right], \tag{12}$$

$$a'(\omega) = a_r' \cos\phi_a + a_i' \sin\phi_a, \tag{13}$$

$$\phi_a''(\omega) = \frac{1}{|a|}\left[a_i'' \cos\phi_a - a_r'' \sin\phi_a - 2a'\phi_a'\right], \tag{14}$$

$$a''(\omega) = a_r'' \cos\phi_a + a_i'' \sin\phi_a + |a|\left(\phi_a'\right)^2, \tag{15}$$

$$\phi_a'''(\omega) = \frac{1}{|a|}\left[a_i''' \cos\phi_a - a_r''' \sin\phi_a + |a|\left(\phi_a'\right)^3 - 3a''\phi_a' - 3a'\phi_a''\right]. \tag{16}$$

Here a' and a'' are taken to be with respect to the magnitude, as in $a'(\omega) \equiv \mathrm{d}\,|a(\omega)|\,/\mathrm{d}\omega$. The expressions above are enough to compute up to TOD, though it is simple to continue to higher order terms as necessary. Making the substitutions $\cos\phi_a \to a_r/|a|$ and $\sin\phi_a \to a_i/|a|$ and simplifying

the results yields compact expressions for the first two phase derivatives,

$$\phi_a'(\omega) = \frac{1}{|a|^2}\big[a_i' a_r - a_r' a_i\big], \tag{17}$$

$$\phi_a''(\omega) = \frac{1}{|a|^2}\Big\{\big[a_i'' - 2a_r'\phi_a'\big]a_r - \big[a_r'' - 2a_i'\phi_a'\big]a_i\Big\}. \tag{18}$$

After solving, in the same manner, for the first m derivatives of $\phi_b(\omega)$, one then substitutes the results into (4) to find the final dispersion terms.

3. Constant Coupling Approximation

To see how one might speed up the algorithm discussed in Section 2.A, consider the specific transfer matrix for a single layer,[7]

$$\mathbf{T}_\ell(\omega) = \begin{pmatrix} \big[1 + p_\ell(\omega)\big]e^{-i\tilde{n}_\ell(\omega)d_\ell\omega/c} & \big[1 - p_\ell(\omega)\big]e^{-i\tilde{n}_\ell(\omega)d_\ell\omega/c} \\ \big[1 - p_\ell(\omega)\big]e^{i\tilde{n}_\ell(\omega)d_\ell\omega/c} & \big[1 + p_\ell(\omega)\big]e^{i\tilde{n}_\ell(\omega)d_\ell\omega/c} \end{pmatrix}, \tag{19}$$

and its first derivative

$$\mathbf{T}_\ell'(\omega) = \begin{pmatrix} \Big\{-id_\ell/c\big[1 + p_\ell(\omega)\big]\big[\tilde{n}_\ell(\omega) + \omega\tilde{n}_\ell'(\omega)\big] + p_\ell'(\omega)\Big\}\, e^{-i\tilde{n}_\ell(\omega)d_\ell\omega/c} & \dots \\ \Big\{-id_\ell/c\big[1 - p_\ell(\omega)\big]\big[\tilde{n}_\ell(\omega) + \omega\tilde{n}_\ell'(\omega)\big] - p_\ell'(\omega)\Big\}\, e^{i\tilde{n}_\ell(\omega)d_\ell\omega/c} & \dots \end{pmatrix} \tag{20}$$

where $\tilde{n}_\ell(\omega) \equiv n_\ell(\omega)\cos\theta_\ell$ is the effective index (which takes into account the angle θ of the wave) and $p_\ell(\omega)$ is the ratio

$$p_\ell(\omega) \equiv \begin{cases} \frac{\tilde{n}_{\ell-1}(\omega)}{\tilde{n}_\ell(\omega)} & \text{TE polarization,} \\ \frac{\tilde{n}_{\ell-1}(\omega)n_\ell^2(\omega)}{\tilde{n}_\ell(\omega)n_{\ell-1}^2(\omega)} & \text{TM polarization.} \end{cases} \tag{21}$$

Everything in the derivative (20) is a simple multiplication of the transfer matrix with the exception of the $\pm p_\ell'(\omega)$ terms which break the symmetry. Fortunately, it turns out that neglecting the derivatives of $p_\ell(\omega)$ is a physically valid approximation for most situations. In the framework of the coupled mode theory used to analyze chirped mirrors,[8] the coupling coefficient κ is proportional to the Fresnel reflection. Thus, taking $p_\ell'(\omega) \to 0$ is equivalent to assuming constant coupling between forward and backward waves. This is discussed further in Section 4.

The resulting reduction in computational complexity from neglecting $p_\ell'(\omega)$ is rather dramatic. Taking the kth derivative of the ℓth transfer matrix is then equivalent to left multiplying the matrix with a trivial operator $\hat{D}_\ell^{(k)}$:

$$\begin{aligned} \mathbf{T}_\ell^{(k)}(\omega) &\approx \hat{D}_\ell^{(k)}\mathbf{T}_\ell, \\ &\equiv \begin{pmatrix} D_\ell^{(k)} & 0 \\ 0 & D_\ell^{(k)*} \end{pmatrix}\mathbf{T}_\ell, \end{aligned} \tag{22}$$

where $D_\ell^{(k)}$ is a complex scalar. Due to the symmetry of transfer matrices, this operator is computationally equivalent to a simple scalar multiplication as opposed to a full matrix multiplication. (In practice, second and higher order derivatives of $\tilde{n}(\omega)$ can be ignored, as well, as they will be small

compared to the error already inherent in the approximation.) The first three matrix derivatives given in (6) can now be written

$$\frac{\partial \mathbf{T}_{(\ell,0)}}{\partial \omega} = \hat{D}_\ell^{(1)} \mathbf{T}_{(\ell,0)} + \mathbf{T}_\ell \mathbf{T}'_{(\ell-1,0)}, \tag{23}$$

$$\frac{\partial^2 \mathbf{T}_{(\ell,0)}}{\partial \omega^2} = \hat{D}_\ell^{(2)} \mathbf{T}_{(\ell,0)} + 2\hat{D}_\ell^{(1)} \mathbf{T}_\ell \mathbf{T}'_{(\ell-1,0)} + \mathbf{T}_\ell \mathbf{T}''_{(\ell-1,0)}, \tag{24}$$

$$\frac{\partial^3 \mathbf{T}_{(\ell,0)}}{\partial \omega^3} = \hat{D}_\ell^{(3)} \mathbf{T}_{(\ell,0)} + 3\hat{D}_\ell^{(2)} \mathbf{T}_\ell \mathbf{T}'_{(\ell-1,0)} + 3\hat{D}_\ell^{(1)} \mathbf{T}_\ell \mathbf{T}''_{(\ell-1,0)} + \mathbf{T}_\ell \mathbf{T}'''_{(\ell-1,0)}, \tag{25}$$

where the scalar factors in (22) are

$$D_\ell^{(1)} = -i\frac{d_\ell}{c}\left[\tilde{n}_\ell(\omega) + \omega\tilde{n}'_\ell(\omega)\right], \tag{26}$$

$$D_\ell^{(2)} = -\frac{d_\ell}{c}\left\{2i\tilde{n}'_\ell(\omega) + \frac{d_\ell}{c}\left[\tilde{n}_\ell(\omega) + \omega\tilde{n}'_\ell(\omega)\right]^2\right\}, \tag{27}$$

$$D_\ell^{(3)} = i\frac{d_\ell^2}{c^2}\left[\tilde{n}_\ell(\omega) + \omega\tilde{n}'_\ell(\omega)\right]\left\{6i\tilde{n}'_\ell(\omega) + \frac{d}{c}\left[\tilde{n}_\ell(\omega) + \omega\tilde{n}'_\ell(\omega)\right]^2\right\}. \tag{28}$$

For a given derivative of $\mathbf{T}_{(\ell,0)}$, all the terms on the right hand side of (23) are trivial operations on previously computed matrices except for one; the sole new term which must be computed is always $\mathbf{T}_\ell \mathbf{T}^{(k)}_{(\ell-1,0)}$. As such, finding the first m derivatives can now be done with $O[nm]$ matrix multiplications, the same complexity of numerical differentiation methods. Moreover, in practice, this analytic computation can be done significantly faster than finite differences since all matrices involved are evaluated at a single frequency and so only one new full transfer matrix must be computed per layer. Since computing a zeroth-order transfer matrix involves costly transcendental operations, this is a significant advantage (see the results in Section 5).

This scheme is still an analytic computation which exactly takes structural and material dispersion effects into account, but which neglects wavelength variation of the coupling between forward and backward waves. For reasonable values of Δn and material dispersion this results in very small errors (as shown in the following section). In cases where group delay is dominated by structural effects, such that local material dispersion can be ignored, this approximation becomes exact.

4. Accuracy of Constant Coupling Approximation

Empirically, we have found that the constant coupling approximation discussed in the preceding section works well for computing at least second order dispersion for any mirror. Moreover, there is theoretical reason to believe that this should be the case, especially for the chirped structures used in dispersion compensating mirrors. Using results from the theory of double chirped mirrors developed by Kärtner and Matuschek,[9,10] we show that the constant coupling assumption is physically justified. This is supported by results from a computation on an actual chirped mirror design.

It is well known that a dielectric stack can be modeled using coupled-mode theory.[8] In this context, the local coupling coefficient $\kappa(\omega)$ is approximately proportional to the Fresnel reflection

between layers:

$$\kappa(\omega) \approx -2r(\omega) = -2\frac{1-p(\omega)}{1+p(\omega)}, \tag{29}$$

where we have dropped the ℓ subscript for this section. Thus, setting $p'(\omega) = 0$ is tantamount to assuming that $\kappa'(\omega) = 0$. Matuschek showed that a chirped mirror can be transformed into a weakly-inhomogeneous coupled-mode problem which can then be solved using the WKB approximation. The group delay of a chirped mirror is then found to be (c.f. equation (52) in Ref. 8)

$$\tau_g(\omega) = -2\int_0^{m_t(\omega)} \frac{\partial}{\partial\omega}\sqrt{\delta^2(m) - \kappa^2(m)}\,\mathrm{d}m, \tag{30}$$

where m is a normalized spatial variable which parameterizes location within the mirror, $m_t(\omega)$ is the location of the classical turning point, and $\delta(m)$ is the coupled-mode detuning coefficient. Matuschek argues that in the classically accessible region of the mirror, the detuning coefficient dominates the coupling coefficient and so, to zeroth order, we have

$$\begin{aligned}\tau_g^{(0)}(\omega) &= 2\int_0^{m_t(\omega)} \frac{\partial}{\partial\omega}\left|\delta(m)\right|\,\mathrm{d}m, \\ &= 2\pi\int_0^{m_t(\omega)} \frac{1}{k_B}\,\mathrm{d}m.\end{aligned} \tag{31}$$

Finally, if the Bragg wavelength k_B is taken to first order as

$$k_B(m) = k_0 + k_1 m, \tag{32}$$

then the group delay can be found analytically to be approximately

$$\tau_g^{(0)}(\omega) = \frac{2\pi}{ck_1}\left[\ln\left(1 - \frac{\kappa(\omega)}{\pi}\right) + \ln\left(\frac{ck_0}{\omega}\right)\right]. \tag{33}$$

The contribution of $\kappa(\omega)$ to the group delay will be minor for $r \ll 1$. Furthermore, $\kappa'(\omega)$ only appears in GDD or higher. Thus, we would expect that neglecting $p'(\omega)$ would be a good approximation for GD, with fair but decreasing accuracy for higher orders of dispersion. This is borne out in the examples shown in Figure 2. Despite its lack of appearance in (33), neglecting $\kappa'(\omega)$ is still only approximately correct for GD due to approximations made in going from (30) to (31).

This can all be understood intuitively by recognizing that the effective round trip optical path length is dominated by the material indices and the location of the classical turning point, the latter of which is not strongly affected by the Fresnel reflection coefficient, $r(\omega)$. This is the case even when the material dispersion itself is large such that local index derivatives must be considered. This can be seen from the GD curve in Figure 2 (a), where neglecting $n'(\omega)$ is shown to be a poor approximation compared to simply neglecting $p'(\omega)$ alone. Thus, despite the fact that $p'(\omega)$ and $n'(\omega)$ are of the same order and both appear in (20) to the same order in ω (since $c/d_\ell \sim \omega$), it is only necessary to consider $n'(\omega)$ when computing $\phi'(\omega)$.

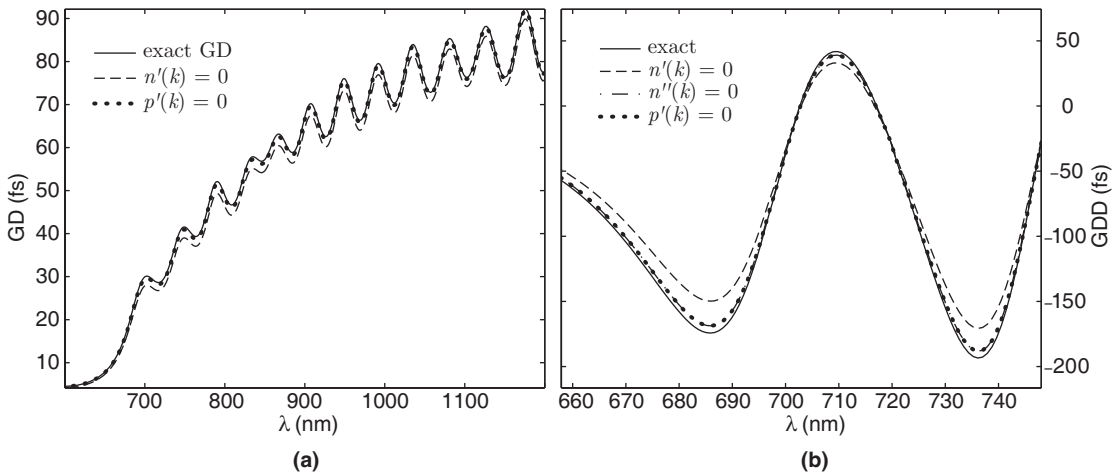

Fig. 2. (a) GD of chirped mirror computed under various approximations. (b) GDD of same mirror under various approximations.

Table 1. Relative execution times under various approximations.

m	Exact	$p'(k) \to 0$	FD
0 (Γ)	1	1	1
1 (GD)	2.45	1.20	2.00
2 (GDD)	4.36	1.42	3.00

5. Example Computations

To gauge the calculation speed of different approximations for various orders of dispersion, we computed the dispersion of off-axis reflection from one half of a double-chirped mirror pair having 80 layers with material indices of roughly 2.5 and 1.4, evaluated at an angle of incidence of 5 degrees. Such mirrors are used for the construction of octave-spanning femtosecond laser systems emitting sub-two-cycle pulses.[2,3] The results for several different cases are shown in Table 1.

Note that the execution time for the exact case increases quadratically with dispersion order whereas that of the constant coupling approximation grows linearly, as predicted in Section 3. Moreover, the constant coupling approximation grows slower than the standard finite difference scheme due to the avoidance of further transcendental function evaluations for higher orders, taking roughly 60% of the time for GD and only 47% for GDD.

To show the effects of the different approximations, we have plotted the GD and GDD for the

double-chirped mirror under various levels of approximation. Figure 2 (a) shows the GD computed exactly, with constant coupling, and with all material dispersion ignored (i.e. $n'(\omega) \rightarrow 0$). Note that the dotted curve representing the constant coupling approximation is virtually indistinguishable from the exact analytic computation. This demonstrates the validity of the approximation even in cases where material dispersion is significant. We have also investigated situations where one material has anomalous dispersion (results not shown here) and obtained similar accuracy.

In Figure 2 (b) we have done the same for GDD and, in addition, have also computed the dispersion assuming second order index derivatives are zero, as well. This result confirms that index dispersion need only be considered to first-order in typical cases. The material system used (SiO_2 and TiO_2) is dispersive enough and the index contrast is high enough such that this example should provide a conservative estimate of the validity of the various approximations.

6. Summary

We have demonstrated an inductive method for exactly computing dispersion of an n layer structure to mth order. This method is, in general, $O[nm^2]$ in time and $O[m]$ in memory. We then introduced an approximation which results in $O[nm]$ execution time, and results in significant speed advantages over even finite differences in practice. The approximation is shown to be adequate for evaluation of GD and GDD.

MATLAB code implementing the algorithms discussed in this paper have been made available on the Internet at *http://rleweb.mit.edu/birge*.

Acknowledgments

The authors would like to thank Christian Jirauschek for helpful discussions. This work was supported by the ONS and the AFOSR.

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