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Robust optimization of adiabatic tapers for coupling to slow-light photonic-crystal waveguides

Ardavan Oskooi,1,* Almir Mutapcic,2 Susumu Noda,1 J. D. Joannopoulos,3 Stephen P. Boyd,4 and Steven G. Johnson5

1Department of Electronic Science and Engineering, Kyoto University, Kyoto 615-8510, Japan
2Sarajevo School of Science and Technology, Sarajevo 71000, Bosnia and Herzegovina
3Department of Physics, Massachusetts Institute of Technology, Cambridge MA 02139, USA
4Department of Electrical Engineering, Stanford University, Stanford CA 94305, USA
5Department of Mathematics, Massachusetts Institute of Technology, Cambridge MA 02139, USA

*oskooi@qe.kuee.kyoto-u.ac.jp

Abstract: We investigate the design of taper structures for coupling to slow-light modes of various photonic-crystal waveguides while taking into account parameter uncertainties inherent in practical fabrication. Our short-length (11 periods) robust tapers designed for $\lambda = 1.55$ $\mu$m and a slow-light group velocity of $c/34$ have a total loss of $< 20$ dB even in the presence of nanometer-scale surface roughness, which outperform the corresponding non-robust designs by an order of magnitude. We discover a posteriori that the robust designs have smooth profiles that can be parameterized by a few-term (intrinsically smooth) sine series which helps the optimization to further boost the performance slightly. We ground these numerical results in an analytical foundation by deriving the scaling relationships between taper length, taper smoothness, and group velocity with the help of an exact equivalence with Fourier analysis.

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1. Introduction

In this paper, we combine large-scale optimization, an increasingly popular tool in nanophotonics [1–16], with robustness and slow light for the problem of coupling two dissimilar waveguides [17–36]: here, a conventional dielectric waveguide and a periodic waveguide with a “slow-light” band edge [37–39] where the group velocity approaches zero. We start with the basic idea of an “adiabatic taper,” a gradual transition that allows wide-bandwidth efficient coupling [40], and apply optimization (∼ 1000 parameters) to design the best “profile” of the taper rate for a given taper length $L$, in order to minimize the tradeoff between taper length $L$ and taper reflectivity $R$. We obtain < 20 dB reflection for $L$ of only a few periods, but we show that the problem becomes intrinsically more difficult as the group velocity decreases, and the resulting optimized designs become more and more counterintuitive. A key idea in our approach is the use of robust optimization [41–45]: optimization that takes into account manufacturing uncertainty (e.g. fabrication disorder or errors in the dielectric constant or operating frequency) by always optimizing the worst-case perturbation to any design. Building on our previous work [43], we show that traditional “nominal” optimization (i.e., assuming no uncertainty) in photonic devices such as this one can easily lead to disaster: an optimized device that performs well only because of some delicate interference cancellation, and whose performance advantage is destroyed even by tiny manufacturing errors. In contrast, the robust optimum degrades much more gracefully in the presence of errors: by taking into account the possibility of errors from the beginning, the robust optimization procedure tends to avoid designs that rely on delicate cancellations. Rather than expensive simulations of the full Maxwell equations performed during the optimization procedure [18,20,21,25,34–36], rapid semi-analytical coupled-mode theory (CMT) [40] calculations are possible for the taper-design problem [37,43]—these initially perform small Maxwell simulations only for the periodic building blocks of the taper to determine the waveguide modes, and subsequently compute a simple integral (equivalent to a weighted Fourier transform) to find the reflectivity of any given taper profile. CMT trades off efficiency for generality, but is an indispensable tool to make large-scale optimization feasible for gradual tapers, especially in 3d. We find that, in the CMT context, the robustness helps us in another way: by comparison to brute-force scattering-matrix calculations [46], we find that our designs are also robust to computational approximations. Even with robustness, however, as the group velocity becomes lower we show that large-scale (many-parameter) optimization tends to push towards an artificial solution that exaggerates discrepancies between the optimization model and the physical circumstances (e.g. modelling errors and/or imperfect uncertainty models), a tendency that can be combatted by building in a posteriori observations about the nature of the robust optima. In particular, we observe that the robust optima tend to be smooth, slowly-oscillating shapes that can be parameterized as a linear taper plus a truncated sine series with a few terms, and by using this information a priori, in addition to robust optimization, we obtain...
Fig. 1. Schematic taper design problem, with a transition between two waveguides characterized by a dimensionless parameter $s \in [0, 1]$. The taper goes from a uniform dielectric waveguide ($s = 0$) to a periodic waveguide ($s = 1$), with $0 < s < 1$ describing intermediate structures (e.g. $s \sim$ hole radius, flange width, or block spacing in the structures shown at right). A taper design (bottom) is a “shape” function $s(z/L)$ (for $z \in [0, L]$) describing a continuous transition from $s(0) = 0$ to $s(1) = 1$. For optimization, we parameterize $s$ by its values at uniformly spaced points and linearly interpolate in between (bottom left).

an improved design at very low group velocities. Although we show analytically that smoothness reduces taper reflections asymptotically for long tapers, the desirability of smoothness for optimized short tapers is not as apparent, especially in light of many previous coupler designs employing abrupt transitions [20, 23, 25, 26, 30, 33, 34, 47, 48].

The coupling of optical modes from one structure to another is crucial for enabling complex integrated photonic devices. A particular challenge is posed by slow-light waveguides, which are useful since their low group velocity enhances many types of light-matter interaction [39] as well as enhancing dispersion effects [37]. For example, the slow-light increase of the field intensity boosts the optical force in optomechanical systems [49–51], and it also enhances nonlinear effects for a variety of applications [39, 52–54]. Many designs have been proposed for coupling dissimilar waveguides (in most cases at moderate group velocities), including designs based on butt-coupling [23, 26], mode-field matching [20, 25, 30, 47], anti-reflection coatings [33, 34], resonant transmission [48], and gradual taper transitions [17–19, 21, 22, 24, 27–29, 31, 32, 36, 37, 40, 43]. Most of these works involved only a small number of tunable degrees of freedom, which (combined with the moderate group velocities) helped to avoid the ultra-sensitive nonmanufacturable designs that tend to arise when many degrees of freedom are included; hence, they were able to disregard uncertainties during
the design process. Resonance can be used to couple to slow light, but is intrinsically narrow-band and relies on a delicate cancellation represented by a forced impedance matching (although, being a single parameter, manufacturing errors could conceivably be compensated by post-fabrication tuning) [48]. Strong frequency and parameter sensitivity was also encountered in the optimization of a coupler over many degrees of freedom [7]. To address a similar problem in our earlier work, we introduced one simple way of incorporating robustness by optimizing the worst-case performance over a large (±30%) range of rescaled taper lengths for the same shape [37]. In particular, we designed an adiabatic taper for coupling to a slow-light 3d flanged waveguide (with a moderately low group velocity of \( c/10 \)) having low reflection (< 20dB), and optimizing over shapes parameterized by a few parameters (degree-4 polynomials) [37]. However, it is desirable to develop a framework in which more general uncertainties can be incorporated. To this end, we recently demonstrated a method for designing waveguide tapers that takes into account uncertainties in the operating frequency and taper shape while using a large number (hundreds) of free parameters [43]. As a proof of concept, we designed a fixed-length (30 periods) taper (to periodic 2d blocks) by smoothly varying the air gaps, coupling to a mode at a moderate group velocity of \( c/4 \) [43]. Here, we extend that work to a more realistic waveguide taper (a waveguide with periodic side flanges, which can be gradually extended while avoiding arbitrarily narrow air gaps), closely analogous to the fabricatable [55–57] 3d flanged waveguide considered in Ref. 37, but in two dimensions so as to be amenable to brute-force validation of its performance in the face of fabrication imperfections (surface roughness). Furthermore, rather than looking at a fixed taper length as in our previous works, we investigate the central engineering tradeoff in this problem: the tradeoff between performance and taper length, by comparing separately-optimized structures at different lengths. We go down to a group velocity of \( c/34 \), where the taper problem becomes even more challenging (both physically and in the optimization sense, e.g. we find that low group velocity required more algorithmic effort to avoid being trapped in poorly-performing local optima, and also requires more care to maintain the validity of CMT). Finally, we extend the asymptotic analysis of the adiabatic limit (taper length \( \rightarrow \infty \)) from our previous works [37, 40] to address the interplay between taper smoothness, group velocity, and reflection (with the help of an exact equivalence to Fourier analysis that we derive here).

In a sense, all engineering design is a problem of optimization: choosing some design parameters \( \mathbf{p} \) to optimize some objective \( O(\mathbf{p}) \), possibly subject to some constraints. Large-scale optimization (sometimes called “inverse design”) is simply optimization in the regime where there are many parameters, so many that one cannot easily intuit the form of the solution. (With many parameters, it is crucial that one evaluate the gradient \( \nabla \mathbf{p} O \) analytically, which can be efficiently achieved by an adjoint method [58].) There are many algorithms to solve optimization problems of many different kinds, but robust optimization is not about the choice of algorithm, it is about changing the optimization problem. Instead of solving a nominal optimization like \( \min_{\mathbf{p}} O(\mathbf{p}) \), in which the optimization process assumes that \( O \) is known exactly with no uncertainties, robust optimization techniques transform the problem to incorporate uncertainties. If the uncertainties are described as unknown values \( \mathbf{v} \) in some set \( \mathcal{Y} \) (e.g. the error bars of manufacturing variability), then one way to “robustify” the problem is to optimize the worst case, \( \min_{\mathbf{p}} [\max_{\mathbf{v}} O(\mathbf{p}, \mathbf{v})] \). (There are also other possibilities, such as optimizing the average case, but worst-case optimization benefits from the availability of many practical algorithms [43]. Reference 45 employed a simplified worst-case analysis for a waveguide-design problem, in which the worst of three designs was optimized.) Most previous work on robust optimization focused on “convex” optimization problems [59]—essentially, problems with no suboptimal local minima, which can therefore be efficiently solved exactly. However, design problems in optics, including the taper design problem here, are typically nonconvex: one cannot in general find...
There are two computational challenges: first, solving Maxwell’s equations to obtain \( R \) for any given \( s \), \( v \), and \( L \); and second, solving the optimization problem (1) for \( R_{\text{min}} \). These two questions are related because a very efficient method to compute \( R \) is desirable in order to rapidly explore a large parameter space \((s, v, L)\) during optimization. To address this challenge,
we first review CMT and its application as a numerical method, and also discuss its analytical implications for the asymptotic properties of gradual tapers. We also compare CMT with more “brute-force” simulation algorithms, which are used both for validation of CMT and for post-optimization evaluation of our designs in the face of disorder. Finally, we briefly review the optimization algorithm, which was developed in detail in our previous work [43].

2.1. Coupled-mode theory and the adiabatic limit

In order to compute \( R \), as in our previous work [37, 43] we employ the coupled-mode theory (CMT) developed in Ref. 40. The basic idea is to expand the field in the waveguide in the basis of the Bloch eigenmodes of periodic waveguides—here, the waveguide modes corresponding to the intermediate structure \( s(z/L) \) is used to expand the fields at that \( z \). Abstractly, if the electromagnetic field is \( \psi(z) \) (with \( xy \) coordinates omitted), we write \( \psi(z) = \sum_n c_n(z) \psi_n(z) \exp[i \beta_n(z') dz'] \), where the \( \psi_n(z) \) are the Bloch eigenmodes at \( z \), \( \beta_n \) is the corresponding propagation constant (or wavevector), and \( c_n \) is the expansion coefficient. When this expansion is substituted into the Maxwell equations, a set of coupled ODEs for \( c_n(z) \) is obtained (the “coupled-mode” or “coupled-wave” equations) [40]. In the \( L \to \infty \) limit, the adiabatic theorem states that the expansion coefficients are constants \( [c_n(z) \to c_n(0)] \), while for a finite \( L \) we can apply a slowly varying envelope approximation (SVEA) to compute the corrections to this limit. In the SVEA, assuming we start with a single incident mode \( c_n(0) = \delta_{0i} \), to lowest order in the rate of change one finds that the reflected-wave amplitude \( c_r \) is [40]:

\[
c_r = \int_0^1 du' \sum_k M_k[u(s)] \frac{\Delta \beta_k}{\Delta \beta_{0i}} \psi_n(s)|\psi_{0i}\rangle du'.
\]

Here, \( M_k(s) \) is a coupling matrix element (an overlap integral \( \langle |\psi_i| \cdots |\psi_r| \rangle \)) of the incident and reflected fields with the geometric variation, and \( \Delta \beta_k(s) = \beta_k(s) - \beta_{0i} + 2\pi k/a(s) \) is a phase-mismatch factor between the incident (i) and reflected (r) modes summed over all Brillouin zones (all integers \( k \)). In this paper, the \( M_k \) and \( \Delta \beta_k \) parameters were obtained from a plane-wave-expansion method [64]. In practice, the sum over \( k \) converges rapidly [40] so we only included \( |k| < 3 \). The reflected power is then \( R = |c_r|^2 \). Computation of the gradient \( \nabla_{c_r} R \) is described in Ref. 43. (It is important to contrast this Bloch-mode expansion with older coupled-wave approaches that expand in the basis of uniform waveguide modes of each cross-section, which is ineffective as a semi-analytical technique for strongly periodic structures in which the cross section is rapidly varying [40]. A Bloch-mode basis, on the other hand, experiences no scattering at all from the periodicity itself—it only undergoes intermodal scattering when the periodicity is broken by the taper, and is therefore a rapidly converging basis for gradual taper transitions of periodic structures, including structures whose unit cells contain discontinuities such as air gaps [40].)

In principle, the total loss (1 − transmission) includes radiative scattering in addition to reflection (assuming single-mode waveguides so that there is no other inter-modal reflection). However, the reflected power tends to dominate [40], especially for slow-light modes (low group velocity \( v_g = d\omega/d\beta \)), as can be argued from (2) [37]. First, at a quadratic band edge in a periodic waveguide, \( \Delta \beta \sim v_g (\text{for the } k \text{ term corresponding to modes } \beta = \pi/a \pm \Delta \text{ coupled in adjacent Brillouin zones}) \)—this both decreases the denominator in (2) and decreases the phase mismatch. Second, the modes in coupled-mode theory are normalized to unit power [40], and hence the fields scale \( \sim 1/\sqrt{v_g} \) and there is an additional \( 1/\sqrt{v_g} \) factor in \( M \) for coupling slow-light incident and reflected modes, versus only a \( 1/\sqrt{v_g} \) factor in \( M \) for coupling slow-light incident to non-slow scattered waves [37].

In order to understand the validity of CMT and the precise scaling with group velocity, we must have a better understanding of the adiabatic limit. A particularly elegant approach
is to make a change of variables to transform (2) into a Fourier integral, at which point all of the well-known properties of Fourier transforms can be invoked. Omit the $k$ summation for simplicity (e.g. focus on the dominant $k$ term). The key point is that one generally (with rare exceptions [65]) considers adiabatic transitions in which the incident and scattered modes are never degenerate in $\beta$, so that $\Delta \beta$ is always nonzero. This is certainly true for the case of reflections. The function $x(u) = \int_0^u \Delta \beta_k [s(u')] du'$ is therefore monotonic, and one can invert it to $u(x)$ and change variables $u \leftrightarrow x$. We obtain precisely a Fourier integral:

$$c_r = \int_{-\infty}^{\infty} dx s'(u(x)) \frac{M_k[s(u(x))]_{\Delta \beta_k [s(u(x)]]^2}}{\Delta \beta_k [s(u(x))]^2} e^{i L x},$$

where we are free to extend the integration range since $s' = 0$ outside the taper. As long as $s$ is continuous, so that $s'$ contains no delta functions, this $\rightarrow 0$ for $L \rightarrow \infty$ because $L$ is simply the “frequency” of a convergent Fourier transform. Furthermore, the rate at which $c_r \rightarrow 0$ with $L$ is well known in Fourier theory to depend on the smoothness of the integrand [66,67], which in this case is determined by the smoothness of $s'$ (including the taper endpoints). For example, if $s$ is a simple linear taper with discontinuous slope $s'$ at the taper ends, then the Fourier transform (due to the discontinuity) scales as $c_r \sim 1/L$, hence the reflections go as $1/L^2$ asymptotically [37,40]. More generally, if $s$ has endpoint discontinuities in its $\ell$-th derivative and is otherwise smooth, then $|c_r|^2 \sim 1/L^{2\ell} [66,67]$ (we previously analyzed a related point in the context of PML absorbing boundaries, where the Fourier analog was not so exact [68]). Similarly, the group-velocity scaling depends on the smoothness of $s$. For the case of a linear taper, or any taper with discontinuous $s'$, the reflection goes as $|c_r|^2 \sim |M/\Delta \beta|^2/L^2 \sim 1/(Lv_g^2)^2$, or equivalently we must have $L \sim 1/v_g^2$ to obtain a fixed reflection [37,69]. For smoother tapers, the convergence analysis of the Fourier integral involves integration by parts to apply additional derivatives to $s$ until the discontinuity is reached [66–67], which gives additional $du/dx = 1/\Delta \beta$ factors by the chain rule. Hence, the generalization to a discontinuity in the $\ell$-th derivative is a scaling $|c_r|^2 \sim |M/\Delta \beta|^2/(L \Delta \beta)^{2\ell} \sim (1/v_g^2)/(Lv_g)^{2\ell}$, or $L \sim 1/v_g^{1+2/\ell}$. The consequence of this scaling is that a tradeoff of taper length with group velocity becomes (asymptotically) better for smoother tapers, approaching $L \sim 1/v_g$, and so smoothness—eliminating high-frequency Fourier components—of the taper shape may be especially important for slow light. On the other hand, the optimum taper shape is very different for any given finite $L$ than it is in the asymptotic limit—the rule is not simply “smoother is better,” because smoother tapers also tend to require a larger $L$ to attain the asymptotic $1/L^2$ behavior [68]. Optimization is required to determine the best shape for any finite $L$, especially for short $L$ far from the asymptotic regime.

2.2. Brute-force numerics and validation

CMT, when evaluated to lowest-order as in (2), is asymptotically exact in the limit of gradual tapers, but is only an approximation for the rapid taper transitions that are the goal of optimization because we are neglecting multiple-scattering effects. (Note that our expansion basis is that of Bloch modes [40], so multiple-scattering effects of the periodicity itself are treated exactly; it is only multiple scattering between Bloch modes due to the taper transition that are neglected.) Fortunately, the optimization will also tend to drive the taper shape precisely into the small-$|c_r|$ regime where CMT is accurate. However, to check the performance of our taper designs, we supplement the CMT with a brute-force numerical calculation based on an eigenmode-expansion scattering-matrix method (also called RCWA, the rigorous coupled-wave approximation) via the free CAMFR package [70]. CAMFR is also used as a final check of the robustness of the designs to fabrication errors, since in that method we can incorporate random
surface roughness in the taper (which requires a different coupled-mode theory technique to describe it accurately [71]). In general, we found that the robust-optimization approach produced designs that were robust even in the face of errors in the computational method, whereas we show below that nominal optimization produces designs whose performance is destroyed even by slight changes in the simulation accuracy.

Figure 2(a) shows a linear (forward and backward, double) taper between a uniform waveguide and a sequence of dielectric blocks ($\varepsilon = 12$), for relatively “fast” light ($v_g \approx c/4$) in the TM (out-of-plane $E$) polarization, with excellent agreement between CAMFR and CMT except for very short tapers with reflections $> 10\%$. This structure is convenient for validation [40,43] because its piecewise-constant cross-sections are particularly efficient in CAMFR and allow us to study very long and gradual tapers, but it is relatively difficult to realize experimentally because its tapers involve many extremely narrow air gaps (that must be abruptly merged in practice once the limits of lithographic resolution are reached [72]). In Fig. 2(b), we instead consider a (TE-polarized) case of a waveguide with lateral flanges [55–57] operating close to the band edge where the group velocity is $\approx c/34$. This sort of geometry is experimentally attractive because a gradual taper involves no arbitrarily narrow features, and the TE polarization translates into a TE-like polarization in three dimensions that can be confined by much thinner structures than TM-like polarizations [38]. In this case, however the CMT only begins to converge to the CAMFR results (which we also check against a third numerical method, FDTD [73,74]) for very long tapers, but this is not unexpected. Because of the slow light used here, the reflections are very large ($\sim 40\%$), and the first-order approximation in our CMT is expected to be inaccurate. For slow light, as explained above, a simple linear taper is a poor choice even if the taper can be made quite long: although CMT predicts an asymptotic $1/L^2$ scaling of the reflection, we would need to go to much larger lengths to observe this scaling for slow light. [Unfortunately, CAMFR is far more expensive for the taper in (b) than for the taper in (a), due to the nonconstant cross-sections in the former, while FDTD is also too expensive to simulate a very gradual taper.] As we show below, however, optimizing the CMT in the slow-light case nevertheless yields a (much more counterintuitive) design that performs well even in the brute-force CAMFR check.

2.3. Robust-optimization algorithm

The basic optimization algorithm, as described in Ref. 43, is sequential linear programming (SLP) with a trust-region constraint [75,76]. In order to implement the robustness [the inner max $v$ of (1)], the method uses the gradient $\nabla v R$ to estimate the worst-case $v$ parameters for the current shape $s$ (and in fact accumulates a memory of ten such worst cases over the course of the optimization that it uses for subsequent steps), and thus transforms the continuous max into a discrete “multi-scenario” maximization over a finite set of worst-case candidates [43].

Reference 43 also introduced a technique of “successive refinement”: we gradually increase the number of degrees of freedom (from 1 to 1024, roughly doubling in each step), using the optimized coarser structures as starting points for optimization of the finer structures. This procedure has two benefits: it both increases the robustness of the design (by making it more robust to coarsening the discretization of $s$) and also tends to avoid becoming immediately trapped in local minima (although we cannot guarantee that the final result is a global minimum).

We found that the precise details of the set $\mathcal{Y}$ of uncertainties makes relatively little difference—putting in any robustness tends to force the optimization to avoid delicate cancellations that would be sensitive to any errors. However, some care is required in the case of slow light because of the presence of a band edge beyond which the guided mode no longer exists. As the band edge is approached, any uncertainty $\Delta \omega$ in the operating frequency must be reduced to avoid going past this band edge. In practice, if a fabrication error were to shift
the band edge slightly, an application requiring slow light would have to either adjust the operating frequency accordingly or perform post-fabrication tuning (e.g. by thermally changing the refractive index) in order to keep \(v_g\) fixed. Therefore, to reflect this situation of fixed \(v_g\), we did not include any uncertainty in \(\omega\). However, in order to represent the possibility of error in the phase velocity \((\omega/\beta)\) that could result from such post-fabrication tuning, we instead included an uncertainty \(\Delta L\) in the taper length \(L\) [equivalent to an overall shift in \(\beta\) by (2)]. Since \(\partial \beta / \partial \omega\) diverges as \(v_g \to 0\), we increased the uncertainty in \(L\) (and hence in \(\beta\)) as we decreased \(v_g\)—failing to do this resulted in designs that were overly sensitive to fabrication errors in our simulations. Furthermore, we found that decreasing \(v_g\) made the optimization increasingly susceptible to being trapped in poor local minima—intuitively, the increased reflections in the slow-light regime also increase the number of opportunities for delicate cancellations—and increasing \(\Delta L\) helped to combat this tendency. We also included random perturbations in \(s\) (at each discretized \(s\) point), but we found that this made little difference in the resulting design once \(\Delta L\) was sufficiently large.

3. Results

We now discuss the results of optimizing and simulating taper designs for the two different waveguides of Fig. 2, considering both slow light and moderate group velocities, for both nominal \((\min R)\) and robust \((\min, \max, R\) optimization), with and without introducing “fabrication disorder” (surface roughness) in the simulation (after optimizing).

3.1. Periodic blocks

To begin with, we return to the periodic (period \(a\)) sequence of \(0.4a \times 0.4a\) blocks (dielectric constant \(\varepsilon = 12\) in air) from Fig. 2(a) that we studied in Ref. 43, operating at the same moderate
Fig. 3. Optimization results for taper structure of square blocks (operating TM mode with $v_g = c/4$) from Fig. 2(a), with block spacing as the taper variable (top: linear tapers). (a) Performance of three tapers (linear in green, nominal optimum in blue, and robust optimum in red, with the optimizations performed independently at each length $L$) computed using a brute-force scattering-matrix method (CAMFR [46]) (with no disorder introduced). (b) Performance of nominal taper (optimized independently at each taper length) computed using two different methods (CMT and CAMFR)—the large disparity is due to the nominal optimum relying on a delicate interference cancellation that is destroyed even by the slight numerical differences between the two techniques. (c) Performance of linear, nominal, and robust tapers designed at $L = 50a$ and then rescaled to other taper lengths: the nominal optimum relies on a delicate cancellation that only works close to $L = 50a$. Inset compares CMT and CAMFR for the $L = 20a$ design rescaled to different lengths, and illustrates that the two approaches agree everywhere except at $L = 20a$, where there is a delicate interference cancellation that is inherently irreproducible (non-robust), and at small $L$ where the reflection exceeds 10% (causing CMT to break down). (d) Nominal and robust taper profiles $s(u)$ designed at $L = 50a$: the nominal design is only slightly different from a linear taper, with the slight changes (inset) sufficient to create a delicate reflection cancellation.
group velocity of $c/4$ and coupled to a uniform waveguide of width $0.4a$, which is a convenient test problem because of the ease of comparison with brute-force CAMFR simulation. Unlike our previous work, however, we now perform the optimization of $s$ separately for every taper length $L \in [1, 100]a$, in order to examine the tradeoff of optimal $R_{\text{min}}$ with $L$. We then simulate each of the resulting taper designs in CAMFR in order to verify their performance.

The results are shown in Fig. 3(a), and exhibit a surprising phenomenon: even when no disorder (no roughness) is introduced into the scattering-matrix (CAMFR) calculation, so that in principle it should be modeling exactly the same system as the CMT calculations used during optimization, the nominal optimum exhibits worse performance than the robust optimum (and both are better than a simple linear taper). Mathematically, one would expect that the nominal optimum should always perform at least as well as the robust optimum when the disorder is set to zero, simply because $\max_{s} R(s, \nu) \geq R(s, 0)$. The reason for the behavior in Fig. 3(a) is simple, however: the nominal optimum relies on such a delicate cancellation effect that even the slight difference in simulation accuracy between CAMFR and CMT (both will have simulation errors, but the errors will be different) is sufficient to radically degrade the performance of the nominal optimum, while the robust optimum still performs well. As shown below, when the nominal and robust optima are evaluated in CMT, the nominal performance is indeed slightly better.

This discretization-error degradation in the nominal optimum can be seen in Fig. 3(b), which compares the CMT and CAMFR calculations for the nominal optimum at each $L$. For very short tapers, they make comparable predictions, but once the taper is about $10a$ in length the optimization is able to engineer a delicate cancellation that causes the CMT reflections to suddenly drop by four orders of magnitude (at which point they become limited by numerical errors and cease to improve further). Even the slight difference in discretization error induced by the switch from CMT to CAMFR, however, is enough to destroy this cancellation. (In our previous work, we showed for this structure that the robust optimum remained an order of magnitude better than the nominal optimum even after additional disorder is intentionally introduced into the CAMFR calculation [43]; we consider such disorder in the next section.) The agreement of CMT and CAMFR everywhere except at the point of this delicate cancellation is demonstrated below, using the inset of Fig. 3(c).

Another viewpoint on this delicate cancellation is shown in Fig. 3(c), which considers the design $s$ for $L = 50a$, but then plots the performance of the same taper shape $s(z/L)$ when it is rescaled to other lengths $L$. The nominal optimum performs well only at the design length of $L = 50a$, and its performance immediately degrades to little better than a linear taper shape $s(u) = u$ as soon as it is rescaled to a different $L$—this is a signature of a delicate destructive cancellation in the reflected wave that the nominal optimization forced to occur at $L = 50a$.

The inset compares CMT and CAMFR for a rescaled $L = 20a$ design, and shows that the two agree except at $L = 20a$ where the non-robust cancellation occurs, which is destroyed by slight differences in discretization error as discussed above. In contrast, the robust optimum still performs well even when $s$ is rescaled to lengths $L$ very different from the $L$ where the shape was designed—the robust optimum does not rely on a delicate cancellation that is easily destroyed. (As expected, the nominal optimum at $L = 50a$ is indeed slightly better than the robust optimum at that $L$, when the two are evaluated in CMT with no disorder.) The corresponding taper shapes $s$ are shown in Fig. 3(d): while the robust optimum is a relatively smooth transition that flattens at the ends (reducing the $s'$ discontinuities of a linear taper as might be expected from the asymptotic analysis), the nominal optimum is nearly identical to a linear taper, only deviating by a slight amount (inset) that is apparently tuned to force a reflection cancellation at $L = 50a$.

Finally, we should comment on one other interesting feature of Fig. 3(a): for the robust optimum, the reflections appear to decrease exponentially with $L$ until reaching a “noise floor” around $10^{-6}$ imposed by numerical accuracy limitations. An exponential tradeoff of reflection
with length is the ideal situation that would be attained asymptotically for an analytic taper shape (such as \( s(u) = \tanh(u)/2 + 1/2 \)), due to the exponential convergence of the Fourier transforms of such analytic functions [67, 68], but this requires the taper to have an infinitely long “tail”, and in any case only applies asymptotically for large \( L \). In contrast, optimization seems to attain a similar ideal tradeoff even for small \( L \), even for finite-length tapers, albeit by changing the taper shape as a function of \( L \). (Whereas the linear and nominal tapers show \( 1/L^2 \) scaling.)

### 3.2. Periodic flanges

Next, we consider taper designs to couple to a waveguide with period-\( a \) dielectric (\( \epsilon = 12 \)) flanges in air, as in Fig. 2(b): the flanges occupy 50% of each period, and extend to an outer diameter (flange width) of \( 2a \) from an inner diameter of \( a \) (matching the uniform waveguide). Again, we optimize separately at each \( L \), in this case for \( L \in [11, 20]a \) (shorter than in the previous section, both for computational tractability in brute force verification and also because short tapers are more practical).

To start with, in Fig. 4, we operate at a moderate group velocity \( c/6 \), at a frequency \( \approx 1\% \) below the band edge of the fundamental mode. After optimization, we then simulated the resulting structures in CAMFR, but modified to include disorder: uniform random surface roughness with amplitude \( \in [-10^{-3}, 10^{-3}]a \) (corresponding to \( \approx \) nm-scale surface roughness for operation at \( \lambda = 1.55 \mu m \)) added to each slice (“pixel”) of thickness 0.01\( a \) of the taper. Each result in Fig. 4(a) is the reflection averaged over 50 realizations of surface roughness. The robust optimum is more than an order of magnitude better in performance than the nominal optimum—
again, the nominal optimum is better in the CMT but relies on delicate cancellations that are destroyed by the surface roughness, although the nominal optimum is still slightly better than a simple linear taper. The robust design has reflections of \( \approx 30 \text{ dB} \) for a taper only \( L = 11a \) in length. The reflection improves for longer lengths, but only slowly, and eventually starts to become worse—the reason is that there is a tradeoff introduced by the surface roughness, in that longer tapers are more gradual but also accumulate roughness-induced reflections over a longer length, and eventually the latter effect dominates. The nominal and robust designs for \( L = 13a \) are shown in Fig. 4(b); note that the vertical axis is exaggerated for clarity. The robust \( s(z/L) \) is a fairly smooth taper transition, exhibits some oscillatory behavior that seems hard to guess \textit{a priori} (and \( s \) will become even more counter-intuitive when the group velocity is decreased below). The nominal optimum is even more strange, with some fine cusps appearing in the first few taper flanges that almost certainly \textit{create} reflections, albeit in such a way as to exactly cancel other reflections (e.g. from the taper ends) in the absence of disorder.

Next, we move to a more challenging problem: coupling to the same structure, but at a frequency only 0.01\% below the band edge of the fundamental mode, operating at a group velocity of \( c/34 \). In this case, a simple linear taper exhibits \( > 30\% \) reflections for a taper length \( L = 20a \). In Fig. 5(a), we show the CAMFR simulations of the optimized designs at each \( L \), again modifying the structures to include surface roughness. The robust optimum here exhibits reflections \( < 20 \text{ dB} \), more than an order of magnitude better than the nominal optimum design, which is again only slightly better than a naive linear taper. The robust optimum, in fact, has a dip \( < 40 \text{ dB} \) in its reflections at \( L \in [13, 15]a \), apparently due to some destructive cancellation, but the dip disappears in Fig. 5(b) if we examine the total loss \( (1 – \text{transmission}) \) instead of just the reflections (which still dominate the loss for most \( L \)). Note that the losses again can be seen to \textit{increase} with \( L \), an effect of the increased scattering from roughness along a longer length. In order to obtain the good performance for the robust taper, we found that we needed to increase the amount of uncertainty \( \Delta L \) in the optimization process to a relatively large value \((3a)\), apparently to avoid being trapped in local minima. In fact, the nominal optimization seemed to immediately become trapped in a relatively poor solution, even for the CMT with no uncertainty—as shown in Fig. 5(c), the nominal optimum achieves \( > 20 \text{ dB} \) reflections in the CMT, a performance that is destroyed when switching to CAMFR even with no surface roughness (due to discretization effects alone).

The nominal and robust optimum shapes \( s(u) \) for \( c/34 \) are shown in the lower-left and top-middle panels of Fig. 6 (again with the vertical axis enlarged for clarity). The nominal optimum has even stronger cusps than in the \( c/6 \) velocity case, suggesting even more reliance on cancellations of strong interior reflections. However, even the robust optimum is highly oscillatory, with oscillations even within a single flange. Despite its good performance in the simulations of Fig. 5, this led us to wonder whether the oscillatory shape was somehow an artifact of the choice of parameterization of \( s \). That is, is this merely a local minimum that we were trapped in as a consequence of discretizing \( s \) into piecewise linear (non-smooth) segments (tent functions) and gradually refining? To investigate this question, we repeated the robust optimization with an entirely different parameterization: \( s(u) = u + (\text{sine series}) \), where the sine series enforces the \( s(0) = 0 \) and \( s(1) = 1 \) boundary conditions. (The \( 0 \leq s \leq 1 \) boundary conditions were imposed explicitly at 1000 points in \( u \), which takes the form of a simple linear constraint added to the linear-programming steps.) Successive refinement was performed by repeatedly doubling the number of terms in the sine series \((4, 16, 32, 64)\), setting the new terms to zero as the starting point for optimization. The resulting robust sine-series optima are shown in Fig. 6 (lower-right), and are clearly converging towards the same oscillatory robust optimum. The 64-term sine series \( s(u) \) is superimposed on the original robust optimum in the top-middle panel, and can be seen to reproduce even many of the fine features within each flange.
Fig. 5. Optimization results for taper from uniform to flanged slow-light waveguide (operating TE mode with $v_g = c/34$) with flange (outer) width as the taper variable (top: linear tapers). (a) Performance of three tapers (linear in green, nominal in blue, and robust in red, with the optimizations performed independently at each length) computed using a brute-force scattering-matrix method (CAMFR [46]), where surface roughness ($\pm 10^{-3}a$ every 0.01$a$) was introduced, averaged over 50 structures. (b) Same as (a) but with 1–transmission: the inclusion of radiative scattering loss eliminates the optimization-created dip (cancellation) in the reflection losses from (a). As in Fig. 4, the robust optimum greatly outperforms the nominal optimum in the presence of disorder. (c) Even without disorder, the nominal optimum performs poorly in CAMFR compared to CMT: the slight differences in simulation accuracy are enough to spoil the nominal optimum. (d) Same as (a) but with robust optimization using the original (1024-point) piecewise-linear (“tent function”) parameterization (red squares) compared to robust optimization using a sine-series parameterization (cyan) with 4, 16, and 64 terms: the latter is converging towards similar performance as the former, and towards similar structures as seen in Fig. 6, so the robust optimum is not merely a local minimum obtained as a byproduct of the discretization choice.
Fig. 6. Linear, nominal, and robust-optimum taper profiles from the slow-light ($c/34$) optimization of Fig. 5, optimized at a taper length $L = 13a$. Vertical axes are exaggerated for scale; topmost (black) figure shows the robust taper design to scale. Even the robust design shows complicated sub-flange oscillations, but similar oscillations are reproduced independent of the parameterization of the taper design during optimization. Top middle (red): robust design using 1024-point linear interpolation (tent functions). Cyan (bottom/right): robust optimization using sine series with successive increase of the number of series terms. 64-term sine series structure (top right) is similar to tent-function (top middle) structure, and is superimposed on the latter as a dotted cyan curve. Nominal optimum (lower left) has even more radical oscillations, designed to create delicate reflection cancellations (which are spoiled by disorder).

The performance of these sine-series designs, shown in Fig. 5(d), is also converging towards the original robust optimum. In fact, the sine series for some $L$ performs better with only 4 terms than it does with more terms or with the original tent-function results. It may be, therefore, that the most counter-intuitive feature of the (tent or 64-sine) robust designs, the intra-flange oscillations, are an artifact not of the parameterization but of the model. That is, the optimization is driving the design towards a regime in which the accuracy limitations of CMT and/or the uncertainty model (which cannot accurately capture surface roughness in the context of CMT) are being exploited to reduce reflections in a way that is partially spoiled in practice (e.g. in brute-force calculations or in experiments). Although the robust designs still perform well, and it would not have been feasible to perform optimization of long tapers on a more exact model, these accuracy limitations can be further compensated for by building in a priori knowledge of the solution: here, the observation that robust solutions tend to be smooth and slowly oscillatory. (In hindsight, a few-term sine-series basis would have been sufficient to parameterize the robust designs in Fig. 3 and Fig. 4 as well.) Robustness is still required: we have checked that nominal optimization applied to the sine-series parameterization continues to yield significantly worse results. In fact, for the $L = 11a$ 4-term sine-series case where the robust optimum...
performed very well, the nominal optimization is immediately trapped in a local minimum and its reflections stay above 10%.

4. Concluding remarks

We have demonstrated how a rapid, semi-analytical Maxwell solver combined with large-scale robust optimization can be used to design taper structures for slow-light photonic-crystal waveguides with performance markedly better than their non-robust counterparts (nominal optima) in the presence of manufacturing variability. In three dimensions, our semi-analytical CMT approach remains feasible [37], and currently seems to be the only feasible computational method in 3d for optimizing the gradual tapers required in slow-light applications. We have shown that robustness, in addition to compensating for manufacturing uncertainty, can also compensate for limitations of CMT to obtain designs that perform well in practice, even though CMT requires increasingly gradual tapers to be accurate as the group velocity decreases. Because we also find that the robust optima tend to be smooth, slowly-oscillating shapes, by building this information into the parameterization a priori—parameterizing the shape as a truncated sine series with a few terms—we find that even better results can sometimes be obtained (although robust optimization is still important). (This finding is reminiscent of—but does not follow from—our analytical result that smooth shapes, with minimal high-frequency Fourier components of $s'$, reduce reflections in the asymptotic $L \to \infty$ limit.) As the group velocity becomes lower, building in smoothness seems to become more and more important for robustness. Using such an a priori low-dimensional representation has other potential benefits: combined with the efficiency of CMT it opens the possibility of more expensive global optimization approaches. Furthermore, these techniques are easily generalized to taper optimization for other waveguide designs, including in 3d, and other uncertainty models. As robust taper designs are particularly useful for coupling to slow-light modes in realistic experimental settings, they may potentially form a crucial component of complex, reconfigurable and dynamic optomechanical devices.

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