

# Integral Equation Method for 1D Taper Problem

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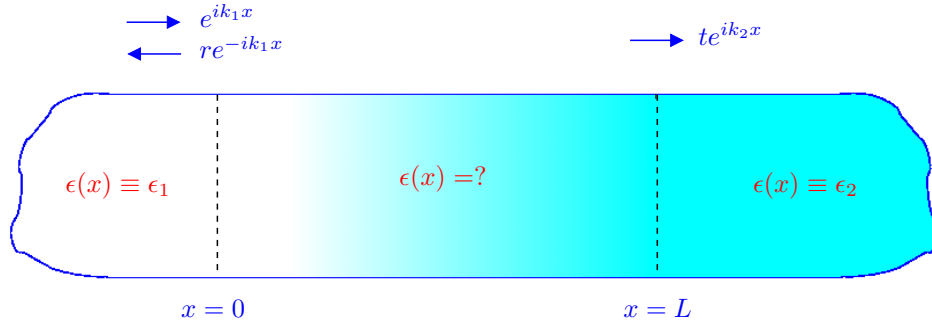


Figure 1: Cartoon depiction of 1D taper problem. Given a trial dielectric function  $\epsilon(x)$ ,  $0 \leq x \leq L$ , we seek to calculate the reflection coefficient  $r$ .

## 1 Overview

We consider the situation depicted in Figure 1. Two media of known dielectric properties are connected by a taper section of length  $L$  and unknown dielectric function  $\epsilon(x)$ . Electromagnetic radiation at frequency  $\omega$  impinges on the taper at  $x = 0$ , is reflected with reflection amplitude  $r$ , and propagates into the medium beyond  $x = L$  with transmission amplitude  $t$ . The goal is to choose  $\epsilon(x)$  so as to minimize the reflected power  $|r|^2$ .

For simplicity in this first exposition, and to emphasize the important general features without needless complications, in this memo we will imagine that the medium beyond the point  $x = L$  is a region of constant dielectric strength  $\epsilon_2$ , so that we are merely tapering between two bulk dielectric media, as illustrated in Figure 1. However, our method works just as well in the case where the region to the right of  $x = L$  is a photonic crystal, with some spatially varying dielectric strength  $\epsilon(x)$ . We will demonstrate this fact in a companion memo[2].

Our presentation is structured as follows:

- In Section 2 we solve Maxwell's equations exactly for the case of a *linear* taper, obtaining exact results for the reflection coefficient.
- In Section 3, building on the results of Section 2, we introduce a systematic solution procedure for solving Maxwell's equations for an *arbitrary* taper.
- In Section 4, we speculate on how the method of Section 3 might allow us to formulate a useful numerical optimization scheme.

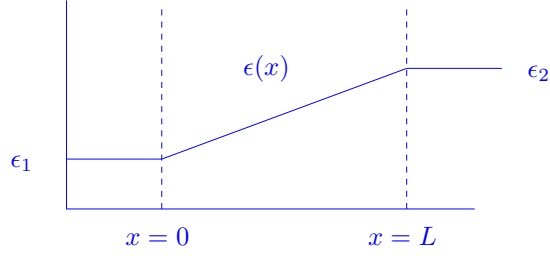


Figure 2: Linearly increasing dielectric taper function considered in Section 1.

## 2 Exact Solution for Linear Taper

We begin by supposing that the dielectric function  $\epsilon(x)$  in Figure 1 rises<sup>1</sup> *linearly* from  $\epsilon_1$  to  $\epsilon_2$ , as illustrated in Figure 2:

$$\epsilon(x) = \epsilon_1 + \frac{\epsilon_2 - \epsilon_1}{L}x.$$

Taking the electric field in the  $y$  direction as before,  $\mathbf{E}(x) = E(x)\mathbf{j}$ , Maxwell's equations amount to

$$\left[ \frac{d^2}{dx^2} + k^2(x) \right] E(x) = 0$$

where

$$\begin{aligned} k^2(x) &= \frac{\omega^2}{c^2} \epsilon(x) \\ &= \begin{cases} k_1^2, & x < 0 \\ k_1^2 + \frac{k_2^2 - k_1^2}{L}x, & 0 \leq x \leq L \\ k_2^2, & L < x, \end{cases} \end{aligned}$$

and

$$k_1 = \frac{\omega^2}{c^2} \epsilon_1, \quad k_2 = \frac{\omega^2}{c^2} \epsilon_2.$$

In the outer regions the electric field is given by

$$E(x) = \begin{cases} e^{ik_1x} + re^{-ik_1x}, & x < 0 \\ te^{ik_2x}, & x > L. \end{cases} \quad (1)$$

On the other hand, in the taper region the field satisfies the differential equation

$$\left[ \frac{d^2}{dx^2} + ax + b \right] E(x) = 0, \quad \left( a = \frac{k_2^2 - k_1^2}{L}, \quad b = k_1^2 \right),$$

<sup>1</sup>Without loss of generality we assume  $\epsilon_2 > \epsilon_1$ .

This is just the Airy equation, with the two linearly independent solutions

$$\text{Ha}(x) = \text{Ai}[-a^{1/3}(x - x_0)], \quad \text{Hb}(x) = \text{Bi}[-a^{1/3}(x - x_0)], \quad \left(x_0 = -\frac{b}{a}\right)$$

where the standard functions Ai and Bi are the solutions to

$$\frac{d^2}{dx^2} \begin{Bmatrix} \text{Ai} \\ \text{Bi} \end{Bmatrix} - x \begin{Bmatrix} \text{Ai} \\ \text{Bi} \end{Bmatrix} = 0.$$

Since Ai and Bi are the Airy functions, we refer to Ha and Hb as the Hairy functions.

The electric field in the three regions is then

$$E(x) = \begin{cases} e^{ik_1x} + re^{-ik_1x}, & x < 0 \\ \alpha\text{Ha}(x) + \beta\text{Hb}(x), & 0 \leq x \leq L \\ te^{ik_2x}, & x > L \end{cases} \quad (2)$$

where  $r$ ,  $\alpha$ ,  $\beta$ , and  $t$  are to be determined by matching the values and derivatives of  $E(x)$  at  $x = 0$  and  $x = L$ :

$$\begin{aligned} E(0^-) &= E(0^+) &\implies & 1 + r = \alpha\text{Ha}(0) + \beta\text{Hb}(0) \\ \left.\frac{dE}{dx}\right|_{0^-} &= \left.\frac{dE}{dx}\right|_{0^+} &\implies & ik_1(1 - r) = \alpha\text{Ha}'(0) + \beta\text{Hb}'(0) \\ E(L^-) &= E(L^+) &\implies & \alpha\text{Ha}(L) + \beta\text{Hb}(L) = te^{ik_2L} \\ \left.\frac{dE}{dx}\right|_{L^-} &= \left.\frac{dE}{dx}\right|_{L^+} &\implies & \alpha\text{Ha}'(L) + \beta\text{Hb}'(L) = ik_2te^{ik_2L} \end{aligned}$$

We thus obtain a 4x4 linear system for the unknown coefficients:

$$\begin{pmatrix} -1 & \text{Ha}(0) & \text{Hb}(0) & 0 \\ ik_1 & \text{Ha}'(0) & \text{Hb}'(0) & 0 \\ 0 & \text{Ha}(L) & \text{Hb}(L) & -e^{ik_2L} \\ 0 & \text{Ha}'(L) & \text{Hb}'(L) & -ik_2e^{ik_2L} \end{pmatrix} \begin{pmatrix} r \\ \alpha \\ \beta \\ t \end{pmatrix} = \begin{pmatrix} 1 \\ ik_1 \\ 0 \\ 0 \end{pmatrix} \quad (3)$$

which we solve readily for arbitrary values of the input parameters.

### Sample results

Figure 3 plots  $|E(x)|$  vs  $x$  for the choice of parameters<sup>2</sup>  $k_1 \cdot L = 10$ ,  $k_2/k_1 = \sqrt{12.9}$ , appropriate for a taper from air into bulk silicon.

<sup>2</sup>Since Maxwell's equations contain no length scale, any one of our dimensionful input parameters ( $k_1, k_2, L$ ) may be chosen arbitrarily and considered a choice of units for our calculations, with only the ratios of the remaining parameters being significant. Thus our calculations here could equally well represent the fields for an  $L = 10 \mu\text{m}$  taper at frequency  $\omega = 3 \cdot 10^{14}$  rad/s, or an  $L = 10 \text{ mm}$  taper at  $\omega = 3 \cdot 10^{11}$  rad/s, etc.

Figure 4 plots the magnitude of the reflection coefficient  $|r|$  for tapers of varying length  $L$  between media of the same dielectric constants as in Figure (3). Evidently  $|r|$  falls off slowly (approximately as  $\sim 1/L$ ) as  $L \rightarrow \infty$ .

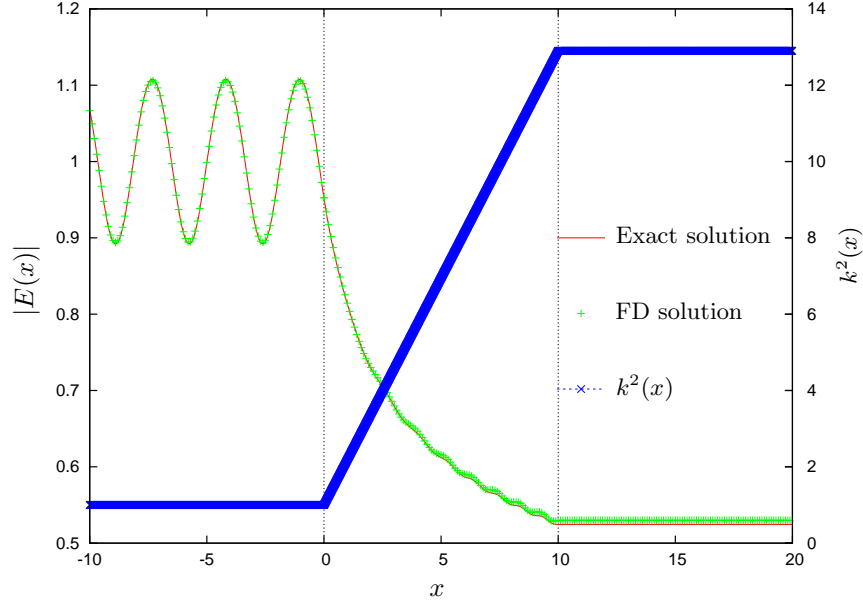


Figure 3: Magnitude of electric field (normalized to unit incident magnitude at  $x = 0$ ) for a linear taper between two constant dielectric media with  $\epsilon_2/\epsilon_1 = 12.9$ . The length of the taper is  $L = 10/k_1$ , where  $k_1$  is the wavevector in the region  $x < 0$ . Solid line: exact solution (equation (1)). Green dots: finite-difference solution, using scattering boundary conditions as outlined in [1], with  $N = 100$  intervals. The slight discrepancy between the solutions for  $x > L$  is due to the roughness of the FD discretization and, we have confirmed, is eliminated entirely at  $N = 1000$ . For reference the function  $k^2(x) \propto \epsilon(x)$  is also shown.

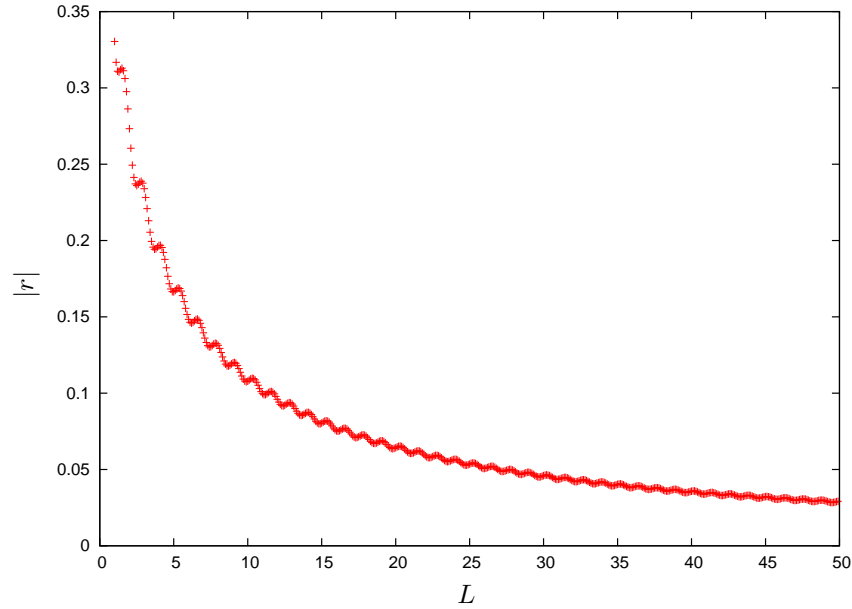


Figure 4: Magnitude of reflection coefficient versus length of taper between the same dielectric media as in Figure 3.

### 3 Systematic Solution Procedure for Arbitrary Taper

#### 3.1 Formulation as an Integral Equation

We next relax the linear-taper assumption and seek to calculate the reflection coefficient for an arbitrary taper function<sup>3</sup>  $k^2(x)$ . To this end, it is convenient to decompose  $k^2(x)$  into a linearly rising term of the type considered previously, which we denote  $k_l^2(x)$ , and a correction term, which we call  $\Delta(x)$ :

$$k^2(x) = k_l^2(x) - \Delta(x), \quad k_l^2(x) = k_1^2 + \frac{k_2^2 - k_1^2}{L}x. \quad (4)$$

The point of this decomposition is that, as we have seen in Figure 4, the linear taper is already optimal in the limit of large  $L$ , so the correction function  $\Delta(x)$ , defined as whatever we need to subtract from  $k_l(x)$  to minimize  $|r|$ , must vanish as  $L \rightarrow \infty$ , i.e.  $\Delta(x) \sim \frac{1}{L} \cdot \Delta_0(x)$  for some universal function  $\Delta_0(x)$ . Then  $1/L$  gives a small parameter in which to do perturbation theory, and, in the apocryphal words of Landau, “theoretical physics *begins* with a small parameter.”

As before, the equation for the electric field is

$$\left[ \frac{d^2}{dx^2} + k^2(x) \right] E(x) = 0.$$

Inserting the decomposition (4), we have

$$\left[ \frac{d^2}{dx^2} + k_l^2(x) \right] E(x) = \Delta(x)E(x). \quad (5)$$

If (5) were homogeneous, i.e. if its RHS vanished, the solution would be simply

$$E(x) = \alpha \text{Ha}(x) + \beta \text{Hb}(x) \quad (\text{homogenous case}), \quad (6)$$

as we saw before. Thinking now of the RHS of (5) as a single source term  $J(x) \equiv \Delta(x)E(x)$ , the solution in the *inhomogenous* case is then simply the *homogenous* solution plus a “forcing” term of the form  $\int G(x, x')J(x')dx'$ , where  $G(x, x')$  is an appropriate Green’s function for the Airy equation. More precisely, the solution of (5) is

$$E(x) = \alpha \text{Ha}(x) + \beta \text{Hb}(x) + \int_0^L G(x, x')\Delta(x')E(x')dx' \quad (7)$$

where  $G$  is the solution to

$$\left[ \frac{d^2}{dx^2} + k_l^2(x) \right] G(x, x') = \delta(x - x'). \quad (8)$$

---

<sup>3</sup>Strictly speaking, the “taper function” is  $\epsilon(x)$ , and we should refer to  $k^2(x) = \frac{\omega^2}{c^2}\epsilon(x)$  as the “position-dependent wavevector squared.” For convenience in what follows we will abuse language by calling  $k^2(x)$  simply the “taper function.”

Equation (7) is a standard integral equation of the second kind with nonsingular integral kernel  $K(x, x') = G(x, x')\Delta(x')$ . One way to think about its solutions is to write

$$\begin{aligned} E(x) = & \alpha\mathbf{H}\mathbf{a}(x) + \beta\mathbf{H}\mathbf{b}(x) \\ & + \int_0^L K_1(x, x') [\alpha\mathbf{H}\mathbf{a}(x') + \beta\mathbf{H}\mathbf{b}(x')] dx' \\ & + \int_0^L K_2(x, x') [\alpha\mathbf{H}\mathbf{a}(x') + \beta\mathbf{H}\mathbf{b}(x')] dx' \\ & + \int_0^L K_3(x, x') [\alpha\mathbf{H}\mathbf{a}(x') + \beta\mathbf{H}\mathbf{b}(x')] dx' + \dots \end{aligned} \quad (9)$$

where the iterated kernels are

$$\begin{aligned} K_1(x, x') &= K(x, x') = G(x, x')\Delta(x') \\ K_2(x, x') &= \int_0^L K(x, x'')K_1(x'', x')dx'' \\ K_3(x, x') &= \int_0^L K(x, x'')K_2(x'', x')dx'' \end{aligned}$$

and so on. Since, as we argued above,  $\Delta \sim 1/L$ , and since each successive iterated kernel contains one more power of  $\Delta$ , the expansion(9) is a power series in  $1/L$ , allowing us to pick off the first-order, second-order, etc. terms in the correction series. If we truncate the series at first order, we obtain an expression for  $E(x)$  that depends *linearly* on  $\Delta(x)$ , giving us a simple linear optimization problem in which we tweak the parameters of  $\Delta$  to minimize the reflection coefficient  $r$ .

Alternatively, a *direct* solution to equation (7) may be obtained by the standard Nystrom method. If  $(\{x_i\}, \{w_i\})$  is an  $N$ -point quadrature rule on  $[0, L]$ , then the vector of E-field values  $E_i \equiv E(x_i)$  is obtained from

$$\mathbf{E} = (\mathbf{1} - \mathbf{K})^{-1} \cdot [\alpha\mathbf{H}\mathbf{a} + \beta\mathbf{H}\mathbf{b}] \quad (10)$$

where the  $N$ -component vectors  $\mathbf{H}\mathbf{a}$ ,  $\mathbf{H}\mathbf{b}$  are defined by

$$\mathbf{H}\mathbf{a}_i = \mathbf{H}\mathbf{a}(x_i), \quad \mathbf{H}\mathbf{b}_i = \mathbf{H}\mathbf{b}(x_i),$$

and the matrix  $\mathbf{K}$  has components

$$K_{ij} = K(x_i, x_j)w_j = G(x_i, x_j)\Delta(x_j)w_j. \quad (11)$$

Having obtained the values  $E_i$  of the electric field at the quadrature points,  $E(x)$  at a general point is evaluated as

$$E(x) = \alpha\mathbf{H}\mathbf{a}(x) + \beta\mathbf{H}\mathbf{b}(x) + \sum K(x, x_j)w_j E_j. \quad (12)$$



Compared to the power series expansion (9), the Nystrom method has the advantage of obtaining at once a full solution for  $E(x)$  in terms of a given  $\Delta(x)$ . Its drawback is that it obscures the dependence on  $\Delta$  in the quantity  $(\mathbb{1} - \mathbf{K})^{-1}$ , making optimization more difficult. (In passing we note that a comparison of the two solution methodologies outlined here leads to an interesting alternative derivation of the Nystrom method itself.)

Whichever of the two solution procedures we choose, before proceeding we must first clear up some loose ends. In particular, we have not said anything about how to choose the values of the arbitrary  $\alpha$  and  $\beta$  coefficients appearing in (7), nor have we specified the appropriate boundary conditions to impose when constructing the Green's function  $G(x, x')$ . The answers to these questions turn out, not surprisingly, to be related to one another, and to motivate these answers we must first take a step backward.

### 3.2 Choice of Constants and Boundary Conditions

To motivate our choice of  $\alpha$ ,  $\beta$ , and the Green's function boundary conditions in (9) (or equivalently in (10)), let's first consider a slightly different problem. Suppose someone simply handed us a function  $E(x)$ ,  $0 \leq x \leq L$ , that described the electric field in the taper region. How would we compute the reflection coefficient given this knowledge?

The answer is that we would proceed exactly as we did in the linear taper case: We would try to match the values and derivatives of  $E(x)$  at the boundaries to the known forms of solutions on the other side of the boundaries. Specifically, we would impose four conditions:

$$\begin{aligned} 1 + r &= E(0) \\ ik_1(1 - r) &= E'(0) \\ te^{ik_2L} &= E(L) \\ ik_2te^{ik_2L} &= E'(L) \end{aligned} \tag{13}$$

and read off the value of  $r$  from the solution.

However, this system has four equations for the two unknowns  $r$  and  $t$ , and hence, to make sense, it must be degenerate: The first two equations must in fact be the same equation, and similarly for the last two. This is only possible if the function  $E(x)$  satisfies certain *internal* constraints, namely,

$$\begin{aligned} E(0) + \frac{1}{ik_1}E'(0) &= 2 \\ E(L) - \frac{1}{ik_2}E'(L) &= 0. \end{aligned} \tag{14}$$

If and only if these conditions are satisfied, the system (13) is solvable and yields the simple solution

$$r = E(0) - 1. \tag{15}$$

This then tells us how to extract the reflection coefficient from our mystery function  $E(x)$ : First verify that  $E(x)$  satisfies conditions (14), and, if so, read off  $r$  from (15).

Let us now apply these ideas to our expression (9) for  $E(x)$ . Our goal is to choose the function  $\Delta(x)$  that minimizes  $r$ , as computed from (15). But any  $\Delta(x)$  we choose must be such as to ensure that the two conditions (14) are satisfied. It turns out this is no limitation on  $\Delta$  at all, because of the two arbitrary constants in (9): Given *any*  $\Delta(x)$ , we could work out all the integrals in (9) with  $\alpha, \beta$  left unspecified, and then at the very end determine  $\alpha$  and  $\beta$  to be as needed to satisfy (14). With  $\alpha$  and  $\beta$  thus determined, we can read off  $r$  for this choice of  $\Delta$  from (15).

This gives an entirely workable scheme. The problem is that it leads to a highly indirect route from  $\Delta$  to  $r$ : Given  $\Delta$ , we must first compute several auxiliary quantities, then solve for the values of  $\alpha$  and  $\beta$  appropriate for this  $\Delta$ , and only *then* read off  $r$ . In other words,  $r$  in this scheme depends on  $\Delta$  in a highly implicit, indirect, and complicated way.

It would be wonderful if we could instead set up our problem so that  $\alpha$  and  $\beta$  were *independent* of our choice of  $\Delta$ . In other words, suppose we could choose  $\alpha$  and  $\beta$  such that equations (14) were satisfied for *any* choice of  $\Delta$ . This would greatly simplify the computation of  $r$  for a given  $\Delta$ , because we could choose  $\alpha$  and  $\beta$  just *once* and then not have to recompute them for each different trial function  $\Delta$ .

Such a feat is indeed possible. The trick proceeds in two steps:

1. Choose  $\alpha$  and  $\beta$  such that (14) is satisfied by the homogenous solution  $E = \alpha H_a + \beta H_b$ , i.e. with  $\Delta$  set to 0; and then
2. Construct the Green's function  $G$  to satisfy boundary conditions such that the inhomogenous term in (7) *does not affect* the satisfaction or otherwise of (14).

In other words, we fine-tune  $\alpha$  and  $\beta$  such that (14) holds, and then ensure that no choice of  $\Delta$  can ever *screw up* that fine-tuning. This has the effect of *decoupling*  $\alpha$  and  $\beta$  from our choice of  $\Delta$ ; it leaves us free to tweak  $\Delta$  at will, looking only at its effect on  $r$ , without worrying that it will ever invalidate (14).

Steps (1) and (2) above are easy to implement. First, we already *know* how to choose  $\alpha$  and  $\beta$  such that (14) is satisfied when  $\Delta = 0$ ; the correct values are simply those that came out of system (3) for the linear taper case. In other words, we choose the homogenous term in (7) to be simply the  $E$  field we obtained for the linear taper back in Section 2. Second, to ensure that the inhomogeneous term in (7) can never screw up the satisfaction of (14), we construct  $G(x, x')$  to satisfy the boundary conditions

$$\left. G(x, x') + \frac{1}{ik_1} \frac{d}{dx} G(x, x') \right|_{x=0} = 0 \quad (16)$$

$$\left. G(x, x') - \frac{1}{ik_2} \frac{d}{dx} G(x, x') \right|_{x=L} = 0. \quad (17)$$

If  $G$  satisfies these conditions, the inhomogenous term in (7) drops entirely out of the consistency conditions (14), leaving their satisfaction or otherwise entirely in the hands of  $\alpha$  and  $\beta$ .

Having identified the boundary conditions  $G$  must satisfy, let us now see how to construct it.

### 3.3 Construction of Green's Function

We seek to construct a function  $G(x, x')$  satisfying equation (8) subject to the boundary conditions (16) and (17). Since this is a pretty standard exercise, we will only survey the essential details. We begin by constructing linear combinations of the Hairy functions that satisfy relations like (16) and (17):

$$f_1(x) = \text{Ha}(x) + \gamma_1 \text{Hb}(x), \quad \gamma_1 = - \left[ \frac{ik_1 \text{Ha}(0) + \text{Ha}'(0)}{ik_1 \text{Hb}(0) + \text{Hb}'(0)} \right]$$

$$f_2(x) = \text{Ha}(x) + \gamma_2 \text{Hb}(x), \quad \gamma_2 = - \left[ \frac{ik_2 \text{Ha}(L) - \text{Ha}'(L)}{ik_2 \text{Hb}(L) - \text{Hb}'(L)} \right].$$

We choose the Green's function to be  $f_1(x')$  to the left of  $x$ , and  $f_2(x')$  to the right of  $x$ , with coefficients chosen in each case to ensure that the value of  $G$  is continuous at  $x' = x$ :

$$G(x, x') = \frac{1}{W} f_1(x_{<}) f_2(x_{>}).$$

Finally, we choose the overall normalization  $W$  to ensure the coefficient of unity on the RHS of (8):

$$\left| \frac{\partial G}{\partial x'} \right|_{x'=x^-}^{x'=x^+} = 1 \quad \implies \quad W = f_1(x) f_2'(x) - f_1'(x) f_2(x).$$

$W$ , being the Wronskian of the solution set of a second-order linear differential equation, is constant, and hence may be evaluated at any convenient point  $0 \leq x \leq L$ .

### 3.4 Sample Results: Optimal Choice of Linear + Sinusoidal Taper

As an illustration of how far we can get by correcting the naive linear taper, suppose we consider a correction term of the form

$$\Delta(x) = \Delta_0 \sin \frac{\pi x}{L}, \quad (18)$$

so that the full taper function is

$$k^2(x) = k_l^2(x) - \Delta_0 \sin \frac{\pi x}{L}.$$

What choice of constant  $\Delta_0$  will minimize the reflection coefficient?

Using the methods of the previous section, we have solved this problem for the parameter values considered previously:  $\epsilon_2/\epsilon_1 = 13.9$ ,  $L = 10/k_1$ . We compute  $|r|$  for various choices of  $\Delta_0$  and seek the optimal value. A plot of  $|r|$  versus  $\Delta_0$  is shown in Figure 5. We find a clear minimum at  $\Delta_0 \approx 3.66$ , at which point the magnitude of the reflection coefficient is reduced to  $|r| = 5.23 \cdot 10^{-3}$ , a improvement by more than a factor of 20 from the value of  $|r| = 0.108$  for the uncorrected linear taper ( $\Delta_0 = 0$ ). Figure (6) shows a plot of  $k^2(x)$  and  $E(x)$  for this optimal case.

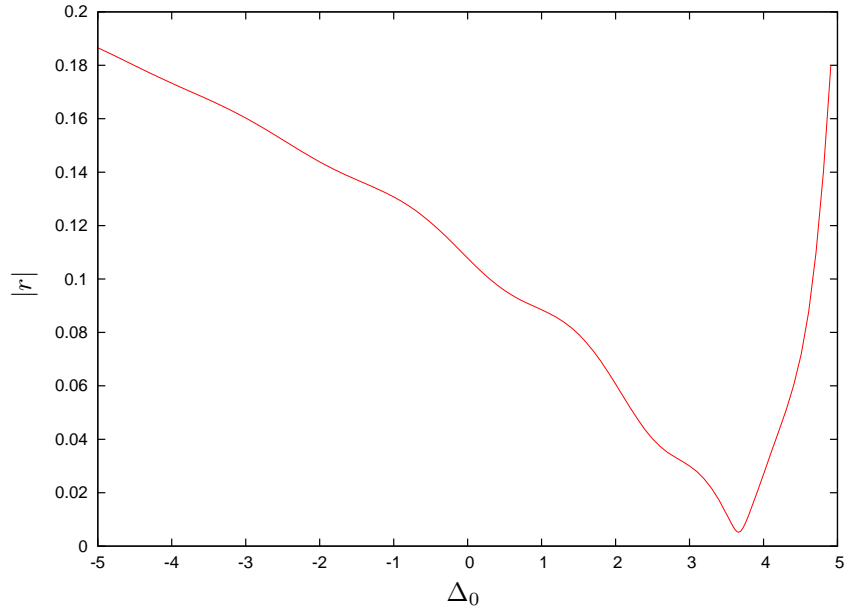


Figure 5: Reflection coefficient versus amplitude of correction term in (18). The minimum of  $|r| = 0.00523$  at  $\Delta_0 = 3.66$  is a 20-fold improvement over the uncorrected value of  $|r| = 0.108$  at  $\Delta_0 = 0$ .

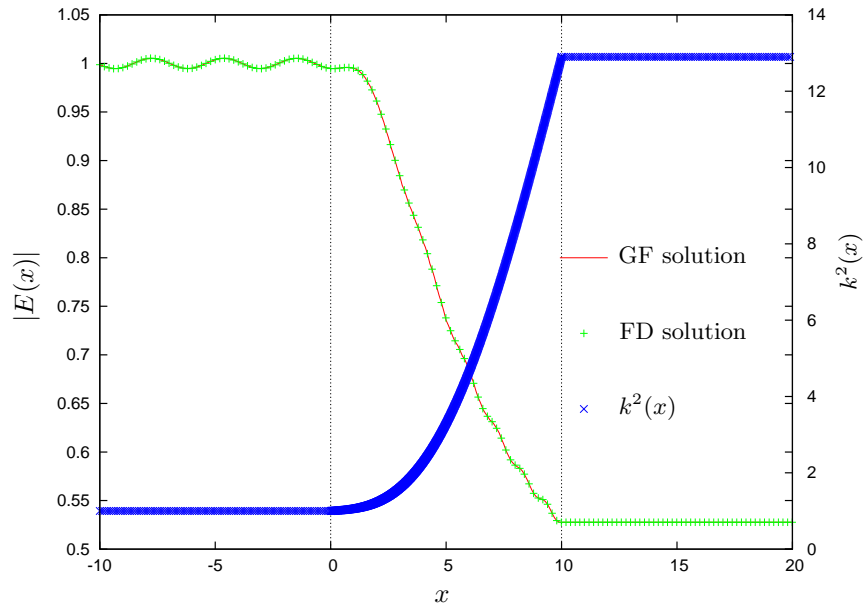


Figure 6: Optimally corrected linear + sinusoidal taper (18), and magnitude of corresponding electric field (normalized to unit incident magnitude at  $x = 0$ ). The reduction in amplitude of the standing wave pattern to the left of  $x = 0$  is clear. (For completeness we have checked our results by computing the fields using the FD method as well).

## 4 Taper Design as a Numerical Minimization Problem

The results of the previous subsection could have been obtained just as easily by the brute-force FD method as by our integral equation technique, so at this point our “method” would appear to be little more than an overly complicated obfuscation of the problem. We believe the virtue of our method to lie in its usefulness as a jumping-off point for various practical optimization schemes, although we admit we haven’t yet devised one. In this section we speculate on a couple of possible directions this jumping-off might take.

### 4.1 Direct Optimization of $\Delta$ at Quadrature Points

One possibility is to take as our optimization variables the set of values  $\{\Delta_i \equiv \Delta(x_i)\}$ , i.e. the taper correction function evaluated at the quadrature points. The starting point for this method is the expansion (9) for  $E(x)$ . Evaluating the integrals by the quadrature rule  $(\{x_i\}, \{w_i\})$ , equation (9) becomes<sup>4</sup>

$$\mathbf{E} = \left\{ \mathbf{1} + \mathbf{K} + \mathbf{K}^2 + \dots \right\} \cdot \mathbf{V} \quad (19)$$

where  $\mathbf{V}$  is the vector of values of the homogenous solution (6) evaluated at the quadrature points,

$$V_i = \alpha \text{Ha}(x_i) + \beta \text{Hb}(x_i),$$

and the matrix  $\mathbf{K}$  is as defined in (11). Using equation (12) in equation (15) and inserting the expansion (19), the reflection coefficient may be expressed as

$$r = \mathbf{U}^\dagger \left\{ \mathbf{1} + \mathbf{K} + \mathbf{K}^2 + \dots \right\} \cdot \mathbf{V} - 1 \quad (20)$$

where the elements of the vector  $\mathbf{U}$  are

$$U_i = G(0, x_i) \Delta(x_i) w_i.$$

We now truncate the expansion in (20) to obtain an approximate nonlinear minimization problem. For example, keeping only the first two terms in the curly brackets leads to the expression

$$r \approx \sum_i x_i \Delta_i + \sum_{ij} y_{ij} \Delta_i \Delta_j - 1$$

where the constant coefficients are

$$x_i = G(0, x_i) w_i V_i, \quad y_{ij} = G(0, x_i) w_i G(x_i, x_j) w_j V_j.$$

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<sup>4</sup>Note that this expansion may equivalently be obtained by Taylor-expanding the matrix inverse in (10).

Squaring, we find

$$r^2 \approx 1 - \sum_i x_i \Delta_i + \sum_{ij} (x_i x_j - y_{ij}) \Delta_i \Delta_j + O(\Delta^3) = \min, \quad (21)$$

a quadratic problem which we minimize by solving a linear system. However, the approximations made in truncating (19) and (21) are in general not justified, so the applicability of this method to the general case is doubtful.

In passing we comment that if we choose a quadrature rule that contains  $x = 0$  as one of our quadrature points, then the value of  $E(0)$  (which we need to compute  $r$ ) is already contained in the vector  $\mathbf{E}$  obtained in (19). In this case the adjoint vector  $U^\dagger$  in (20) is a constant (actually a vector with a single entry of unity and zeros everywhere else) independent of  $\Delta$ , which should simplify an optimization method following these lines.

## 4.2 Expansion of $\Delta$ in Orthogonal Functions

An alternative is to expand  $\Delta(x)$  in some basis of orthogonal functions. Since our construction allows us to take  $\Delta(x)$  to vanish at the endpoints of the taper, we consider, as one example, an expansion of the form

$$\Delta(x) = \sum_{n=1}^N C_n \sin \frac{n\pi x}{L}.$$

The results of Section 3.3 above correspond to the case  $N = 1$ , in which case we found the value  $C_1 = 3.66$  to be optimal. In the general case the vectors and matrices in (20) look like

$$\begin{aligned} \mathbf{U} &= \sum C_n \mathbf{U}^n, \\ \mathbf{K} &= \sum C_n \mathbf{K}^n, \end{aligned}$$

where the  $C_n$ -independent quantities are of the form

$$\begin{aligned} \mathbf{U}_i^n &= G(0, x_i) w_i \sin \frac{n\pi x_i}{L} \\ \mathbb{K}_{ij}^n &= G(0, x_i) w_i G(x_i, x_j) w_j \sin \frac{n\pi x_i}{L} \sin \frac{n\pi x_j}{L} \end{aligned}$$

Inserting into (20), we again obtain a complicated nonlinear optimization problem, but this time in terms of the  $C_n$  coefficients, which in general will be many fewer in number than the  $\Delta_i$  coefficients.

The ideal scenario, of course, would be if we could devise some method of disentangling the  $C_i$  coefficients from one another, perhaps by some clever choice of expansion functions, such that the effect on  $r$  of tweaks to  $C_i$  would be independent of the values of the other coefficients  $C_j$ . The construction of such a scheme, as well as the extension of all of these ideas to three dimensions, are left as exercises for the reader.

## **References**

- [1] H. Reid, previous memo in this series.
- [2] H. Reid, next memo in this series.