14

Wide-Angle Beam Propagation Methods

The beam propagation methods discussed so far, with notable exceptions of spectral propagators, can be characterized as paraxial. However, we have not invoked the paraxial approximation explicitly in the course of the derivation that gave us the beam propagation equations. Yet, analysis of their dispersion properties showed that they are indeed paraxial, and as such they impose incorrect properties on waves propagating at large angles. One can ask where exactly the paraxial approximation appears? In this chapter we will trace this to the uni-directional approximation and the slowly evolving envelope approximation. We will see that while waves propagating in the "opposite" direction need not be included in the simulation, the *possibility* that they occur must be considered during the derivation.

14.1 Padè approximations for propagation operators

This section follows the original treatment by Hadley, who introduced Padè approximation into the BPM field. Padè approximant is a function that approximates given $f(x)$ in terms of a rational function, or ratio of two polynomials of x:

$$f(x) \approx R(x) = \frac{M(x)}{Q(x)} = \frac{\sum_{j=0}^{n_P} m_j x^j}{1 + \sum_{j=1}^{n_Q} q_j x^j} \tag{14.1}$$

The feature that distinguishes this approximation from any other is that the coefficients in the numerator and denominator polynomials are selected such that the Taylor expansion of $f(x)$ is reproduced up to a certain order that is determined by the number of free coefficients. Depending on the order of the polynomials, Padè approximants come in different types. If the order of $M(x)$ and $Q(x)$ are n_M and n_Q, respectively, then the Taylor expansion can be matched up to order $n_P + n_Q$

$$f(0) = R(0) \quad , \quad f'(0) = R'(0) \quad , \dots \; , \; f^{(n_Q+n_M)}(0) = R^{(n_Q+n_M)}(0) \; , \tag{14.2}$$

and such an approximation is called type (n_M, n_Q). Naturally, there are many approximants for the same function, and which is best depends on circumstances. The main reason "Padeization" is so useful in the field of BPM is that it helps to preserve sparsity of various discretized differential operators as we shall see shortly.

Let us first discuss the original Hadley's method in which approximations for beam propagation equations are introduced with the help of a recursion. Consider first a scalar Helmholtz equation for the TE-polarized electric field in a space with a single transverse dimension

$$(\partial_{zz} + \partial_{xx} + k_0^2 n(x)^2)E = 0 \ , \tag{14.3}$$

and let us cast this in terms of the field envelope A,

$$E = e^{ik_r z} A \ , \tag{14.4}$$

where k_r is a reference wavenumber that defines a reference refractive index such that $k_r = k_0 n_r$. Then the envelope equation reads

$$(\partial_{zz} + 2ik_r \partial_z + \partial_{xx} + k_0^2(n^2 - n_r^2))A = 0 \ . \tag{14.5}$$

Denote

$$P = \partial_{xx} + k_0^2(n^2 - n_r^2) \tag{14.6}$$

the transverse portion of the Helmholtz operator. For the TM polarization we would have

$$PA = \frac{\partial}{\partial x}\frac{1}{n^2}\frac{\partial n^2 A}{\partial x} + k_0^2(n^2 - n_r^2)A \ . \tag{14.7}$$

The propagation equation can be in both polarizations put in a form

$$\partial_z(1 + \frac{1}{2ik_r}\partial_z)A = \frac{i}{2k_r}PA \ . \tag{14.8}$$

From here, the usual next step which results the paraxial approach is to neglect the second term in brackets, and this is justified by the large value of k_r. In the wide-angle propagation context, the second derivative w.r.t. z has to be retained. At the same time, one wants to obtain a first-order derivative on the left-hand-side. The equation can be formally solved as follows

$$\partial_z A = \frac{i}{2k_r}\frac{P}{1 + \frac{1}{2ik_r}\partial_z}A \ . \tag{14.9}$$

Of course, the reader should suspect that the expression in the denominator in fact represents an inverse differential operator, and it is not immediately obvious that it exists. It is also not clear how the above operation it represents can be practically calculated. However, imagine that we already have an approximation for how ∂_z acts on A. Then we could try the following recursion suggested by the above equation:

$$\partial z|_n = \frac{iP/(2k_r)}{1 + \frac{1}{2ik_r}\partial_z|_{n-1}} \ , \tag{14.10}$$

and start with

$$\partial z|_0 = \frac{i}{2k_r}P \ , \tag{14.11}$$

which is a natural zero-order approximation, because it generates the well-known paraxial BPM propagation equation. This will initiate a series of approximations for wide-angle beam propagation equations. In the first order, we get

$$\partial z|_1 = \frac{iP/(2k_r)}{1 + \frac{1}{2ik_r}\frac{i}{2k_r}P} \ , \tag{14.12}$$

in order two we have

$$\partial z|_2 = i\frac{P/(2k_r) + P^2/(8k_r^3)}{1 + P/(2k_r^2)} \ , \tag{14.13}$$

and order three yields

$$\partial z|_2 = i\frac{P/(2k_r) + P^2/(4k_r^3)}{1 + 3P/(4k_r^2) + P^2/(16k_r^4)} \ . \tag{14.14}$$

We could continue this way to higher and higher orders, hoping that the process converges in some sense.

From each of these expressions we obtain a propagation equation, for example the last one gives

$$\partial z A = i\frac{P/(2k_r) + P^2/(4k_r^3)}{1 + 3P/(4k_r^2) + P^2/(16k_r^4)} A \ . \tag{14.15}$$

In the second order the propagation equation is

$$\partial z A = i\frac{P/(2k_r) + P^2/(8k_r^3)}{1 + P/(2k_r^2)} A \ , \tag{14.16}$$

and the lowest order coincides with the paraxial propagation equation

$$\partial z A = iP/(2k_r)A = \frac{i}{2k_r}\left[\partial_{xx} + k_0^2(n(x)^2 - n_{\text{ref}}^2)\right] A \ . \tag{14.17}$$

Setting aside the question of how to solve these propagation models, we should first ask if the above procedure really leads to “healthy” propagation equations? Fortunately, all representations that arise in this recursion can be justified with the help of Padè approximants to a “factorized” Helmholtz equation. The latter can be obtained as a formal solution to (14.8):

$$\frac{\partial A}{\partial z} = ik_r\left(\sqrt{1 + P/k_r^2} - 1\right) A \ . \tag{14.18}$$

Substitution and formal manipulation with the square root of an operator indeed shows that if this equation is fulfilled, (14.8) will be satisfied, too. An alternative way to look at this is to write Helmholtz with addition and subtraction of the chosen reference wavenumber,

$$(\partial_{zz} + \partial_{xx} + k_0^2 n(x)^2 - k_r^2 + k_r^2)E \equiv (\partial_{zz} + P + k_r^2)E = 0 \ . \ , \tag{14.19}$$

Inspired by the one-dimensional wave equation, one can factor the above to get

$$(\partial_{zz} + P + k_r^2)E = (\partial_z + i\sqrt{P + k_r^2})(\partial_z - i\sqrt{P + k_r^2})E = 0 \ . \tag{14.20}$$

The two operators in brackets represent waves propagating in opposite directions. Beam propagation along positive z is described by the second factor, so we drop the other. This is where we transition form the original bi-directional propagation system to a uni-directional one. With the electric field represented in the envelope picture, the second factor yields

$$0 = (\partial_z - i\sqrt{P + k_r^2})e^{ik_r z}A \to \partial_z A = ik_r(\sqrt{1 + P/k_r^2} - 1)]A \ , \tag{14.21}$$

which is the equation we sought.

Since in general there is no direct way to evaluate square root of an operator, we will replace it by its Padè approximant(s). For example, type (2,2) Padè approximant of $\sqrt{1+X} - 1$ is

$$\frac{X/2 + X^2/4}{1 + 3X/4 + X^2/16} \ .$$

With $X = P/k_r^2$, and (14.33) this results in equation (14.15). In a similar way, all results obtained from the above recursion can be justified as Padè approximants to the factorized Helmholtz equation in the envelope representation.

What has been achieved so far is the formal separation of the waves that propagate in forward and backward directions. Is is interesting that this eliminates paraxiality from the propagation equations. The calculations of this section tell us that the paraxial approximation appeared in the previous treatment as a consequence of ignoring the *possibility* of wave propagation in the direction opposite to that of the beam.

As a matter of practical importance, we have replaced the quite unyielding operator square root with a Padè approximant resulting in a rational function of the Helmholtz-related operator P. Next we address the question of numerical solution of the wide-angle propagation equations.

14.2 Numerical solution of wide-angle beam propagation equations

Depending on the type of Padè approximation chosen, the corresponding beam evolution equations will differ in details, but their solution is in essence the same. In general the right-hand-side operator acting on the previously calculated beam amplitude is a ratio of two polynomials in $P/(2k)$:

$$\partial_z A = ik \frac{\sum_k n_k (P/2k_r)^k}{\sum_k d_k (P/2k_r)^k} A \equiv ik \frac{N(P)}{D(P)} A \ . \tag{14.22}$$

To obtain a discrete-grid update scheme, take (as usual, upper index labels mark integration steps)

$$\partial_z A \approx \frac{A^{(n+1)} - A^{(n)}}{\Delta z} \ , \tag{14.23}$$

and

$$ik \frac{N(P)}{D(P)} A \approx ik \frac{N(P)}{D(P)} \frac{(A^{(n+1)} + A^{(n)})}{2} \ . \tag{14.24}$$

This is the classic Crank-Nicolson finite-difference scheme. Let us see if all quantities involved can be efficiently calculated. Multiplying by the operator in the denominator yields

$$D(P)(A^{(n+1)} - A^{(n)}) = \frac{ik\Delta z}{2} N(P)(A^{(n+1)} + A^{(n)}) \ . \tag{14.25}$$

Grouping equal-z quantities on one side of the equation, one gets

$$[D(P) - \frac{ik\Delta z}{2} N(P)] A^{(n+1)} = [D(P) + \frac{ik\Delta z}{2} N(P)] A^{(n)} \ . \tag{14.26}$$

The expressions on both sides of this equations are polynomials of P. This is the type of operator function that does not present conceptual difficulties, at least in the finite-dimensional space of discrete solutions that arise in BPM. An important point is that this representation preserves the sparse-matrix nature of operator P.

When it is discretized on the spatial grid, for example the way described in the previous chapter, this update scheme represents a large linear system of equations. The most straightforward approach to its solution is to use a linear solver library. There are, roughly speaking, only two options. The first is to use a direct, sparse-matrix solver the way we have done it in the exercise on the two-dimensional Crank-Nicolson BPM. The task is more difficult in more than one way in this case. First, the resulting matrix of the linear system is more complex, because it contains powers of operator P. The latter is represented by a truly sparse matrix in which only nearest-neighbor grid points are coupled. As higher and higher powers of P arise, further and further neighbors become coupled, and this results in more non-zero elements of the matrix. Moreover, during the process of solution this matrix fills up even more. All this results in higher usage of computer memory. Yet another difficulty is due to a more complicated way to set up the system matrix. If a routine for sparse-matrix multiplication is available, then the total matrix can be conveniently built gradually by adding higher-order terms. If the integration step is fixed, the result can be retained and the computational cost of the initial setup is irrelevant. At any rate, using a direct sparse-matrix solver always requires significant computer memory and this may limit, in practice, the maximal size of the system that can still be simulated.

An alternative approach, which also treats the propagation equation as a linear system of algebraic equations, is to use an iterative solver. Unlike the direct solver, it does not guarantee that a solution will be obtained in certain number of steps, or that a usable solution will be obtained at all. An iterative solver starts from an ansatz solution, an improves on that in a series of iterations. The result is an approximate but usually quite accurate solution. Iterative methods come in several versions, but they all share several features that make them attractive specifically for BPM applications. Most importantly, rather large systems can be solved, because the matrix is never stored explicitly in the computer memory. In fact, there is no need to construct the matrix. Instead, iterative solvers only require that the user provides an algorithm to evaluate the action of the matrix on a given vector, which is supplied by the solver. This is especially convenient in this case; When the solver asks to calculate action of the system matrix on some vector X that was generated during the iterative process, the user must evaluate

$$[D(P) - \frac{ik\Delta z}{2}N(P)]X \ .$$

Because this is a polynomial in P, the result can be obtained by at most $\max(n_D, n_N)$ of multiplications by the matrix representing P. Consequently, the BPM program based on iterative solver is conceptually relatively simple as it only requires to specify an algorithm for the matrix-vector multiplication PX. Very similar is the calculation of the right-hand-side of the linear system that represent one BPM step. It is also evident that the algorithm complexity goes up linearly with the order of the Padè rational function. These issues are illustrated in exercise-package *EP-19*.

14.3 Dispersion relations

Because the scheme introduced in the previous section are all based on the same discretization approach as the classical Crank-Nicolson method, it is natural to expect that they also share the favorable numerical dispersion properties. Namely, they should be unconditionally stable and second-order in the in the integration step length.

To show that this is indeed the case, note that the polynomial functions of operator P that occur in the right- and left-hand-side of the update scheme are closely related. In fact, when written expanded in the polynomial form, they exhibit coefficients that are mutually complex-conjugate. In other word, single update step can be written as

$$A^{(n+1)} = \frac{\sum_{i=0}^{n} \xi_i P^i}{\sum_{i=0}^{n} \xi_i^* P^i} A^{(n)} \ . \tag{14.27}$$

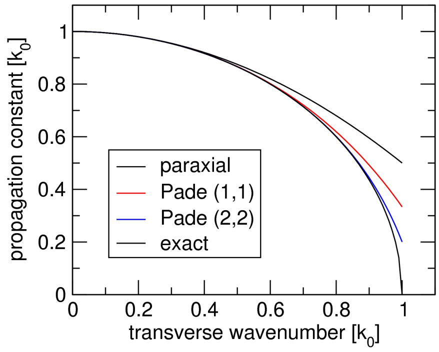
Now, spectrum of P is real, and its eigenvectors constitute a possible basis in the discrete space of beam solutions. One can show the same way as for the paraxial C-N method that propagation constants of these eigenfunctions are all real. That in turn means that the method preserves the norm of the solution and is therefore unconditionally stable, and has no damping.

As for this method‘s accuracy, it is instructive to look closer at concrete dispersion relations. This is only possible when all eigenfunctions of P are known explicitly. For practical purposes, this means a homogeneous medium, which is a very special case, but it does illustrate how increasing Padè order improves wave propagation at wide angles.

Consider a uniform medium with single transverse dimension x, and choose the reference index equal to that of this medium. Plane waves characterized by their transverse wavenumber k are then eigenfunctions of P with eigenvalues $-k^2$. The corresponding propagation constant of the electric field (as opposed to envelope) wave is.

$$\beta(k) = k_0(\sqrt{1 - k^2/k_0^2})$$

To appreciate the difference between the exact and WA-BPM wave propagation *in the continuum limit* (small Δx) it is enough to compare $\beta(k)$ to the chosen Padè approximation. This is shown in the figure in units of the on-axis propagation constant k_0:



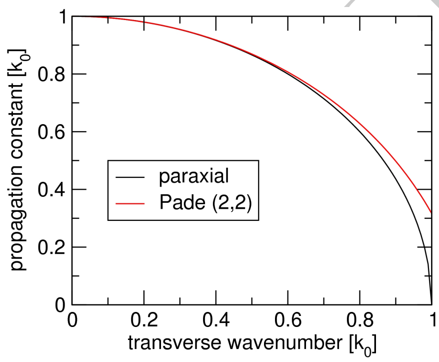
Normalized propagation constant for a plane wave with a given transverse wavenumber calculated for several Padé approximants. This picture corresponds to the continuum limit $\Delta x \to 0$ and shows the best result achievable with a given approximation.

The picture indicates that the gap between approximated and exact propagation constants shrinks rapidly with the increasing order of Padè approximation. In fact, in the continuum limit at least, $(2, 2)$ Padè method propagates correctly waves at angles exceeding forty five degrees.

To appreciate effects of the discrete grid, one has to look at the discrete eigenvalue of P which depends on the grid spacing Δx:

$$\frac{2}{k_0^2 \Delta x^2}[\cos(k\Delta x) - 1] \ .$$

For the following illustration, let us choose $\Delta x = \lambda/(2\pi)$ which represents a decent grid resolution for the propagation in a homogeneous medium.



Normalized propagation constant of the Padè(2,2) approximation compared to the continuum-limit exact case for $\Delta x = \lambda/(2\pi)$. The transverse wavenumbers at which the two curves start to separate decrease even further on a coarser spatial grid.

This picture illustrates that the numerical dispersion increases the deviation from the desired exact propagation constant. One can see that, in comparison with the continuum limit shown in the previous figure, the two curves start to separate at significantly smaller angles of propagation already when $\Delta x = \lambda/(2\pi)$.

14.4 Multi-step method

Wide-angle BPM, even when it is applied in a single transverse dimension, leads to systems of linear algebraic equations that are not tri-diagonal. Consequently, less efficient solvers must be applied, because each subsequent power of operator P adds a new pair of off-diagonal elements. However, the case of one transverse dimension is practically interesting, as it includes modeling of integrated devices in the effective index approximation. Wide angle approach may be often required when waves, while confined to a single 'vertical' guided mode, propagate at large angles within the plane of the device. This motivates the question if it is possible to re-formulate the theory outlined in the previous section in way that would allow utilization of tri-diagonal solvers. The approach that does this is called multi-step, and was first proposed by Hadley. We will initially follow his line of reasoning, and later proceed to generalization.

The basic expression for one propagation step contains related polynomials in P.

$$A^{(z+1)} = \frac{D(P) + \frac{ik\Delta z}{2}N(P)}{D(P) - \frac{ik\Delta z}{2}N(P)}A^{(z)} = \frac{\sum_{i=0}^{n}\xi_i P^i}{\sum_{i=0}^{n}\xi_i^* P^i}A^{(z)} \ . \tag{14.28}$$

Polynomials $N(P)$ and $D(P)$ are obtained from the Padè approximant of $\sqrt{1+P/k_r^2}-1$, and they in turn determine expanded expression on the right. For example, for type $(2,2)$ method we have

$$\xi_0 = 1 \quad , \quad \xi_1 = \frac{2+ik_r\Delta z}{4k_r^2} \quad , \quad \xi_2 = \frac{i\Delta z}{16k_r^3} \ . \tag{14.29}$$

These polynomials can be factorized, and since it is a general property that $\xi_0 = 1$, the factorization can be put in the form

$$\sum_{i=0}^{n}\xi_i P^i = (1+a_nP)\dots(1+a_2P)(1+a_1P) \ . \tag{14.30}$$

Also, because the two polynomials are mutually complex conjugated, the stepping scheme can be written with factorized terms "paired" as in

$$A^{(z+1)} = \frac{(1+a_nP)\dots(1+a_2P)(1+a_1P)}{(1+a_n^*P)\dots(1+a_2^*P)(1+a_1^*P)}A^{(z)} \tag{14.31}$$

This can be implemented as a series of sub-steps

$$A^{(z+i/n)} = \frac{(1+a_iP)}{(1+a_i^*P)}A^{(z+(i-1)/n)} \quad i = 1,2,\dots,n. \tag{14.32}$$

The advantage of this equivalent formulation is that for one transverse dimension each of the intermediate steps is linear in P, and its linear system matrix is tri-diagonal. Consequently, the efficient Thomas algorithm can be used.

One inconvenience of the multi-step method is that coefficients a_i must be obtained from roots of a polynomial in which coefficients depend on the concrete choice of the integration step. There is no general explicit formula to tabulate the general WA-BPM algorithm, and numerical root-finding must be executed every time integration step size changes.

14.5 Padè approximation of evolution operators

What the multi-step method does is in fact an approximation of the beam evolution operator over a distance corresponding to a single step. Coefficient in this rational function are determined in two approximate steps. First, square root of the Helmholtz operator is replaced, and the symmetric discretization scheme of second-order accuracy is applied. One can naturally ask if it is possible to create a numerical evolution operator in a "single step." One possible approach to this problem is what we discuss next.

We start from the uni-directional beam propagation equation

$$\frac{\partial A}{\partial z} = ik_r \left(\sqrt{1 + P/k_r^2} - 1\right) A \quad , \quad P = \Delta_\perp + k_0^2 n^2 - k_r^2 \ , \tag{14.33}$$

and write its solution in the form of an operator exponential

$$A(z + \Delta z) = \exp\left[ik_r \Delta z(\sqrt{1 + P/k_r^2} - 1)\right] A(z) \ . \tag{14.34}$$

This exponential can be approximated by a rational function of P:

$$\exp\left[ik_r \Delta z(\sqrt{1 + P/k_r^2} - 1)\right] \approx \frac{(1 + c_n P) \ldots (1 + c_2 P)(1 + c_1 P)}{(1 + c_n^* P) \ldots (1 + c_2^* P)(1 + c_1^* P)} \ . \tag{14.35}$$

Choosing coefficients in the denominator as complex conjugate of those in the numerator ensures that this operator is unitary, i.e. it preserves the energy (or power) in the propagating beam.

To obtain equations, or constraints, for c_i, one can require that the right hand side is certain Padè approximant of the exact evolution operator. In general, we expand both sides into Taylor expansion and then adjust c_i such that lower-order terms in P are canceled. It is not possible to solve the resulting equations analytically. However, it is possible to obtain useful approximation by looking for some simplified solutions. Solution obtained in this way may not be optimally accurate given the number of degrees of freedom encompassed by the set of coefficients c_i, but have the advantage that adaptive step control is easier because c_i can be expressed as analytic functions of Δz. This approach is illustrated in exercise *EP20-WA-BPM.*

For example, one may parametrize the solution in the following form

$$\exp\left[ik_r \Delta z(\sqrt{1 + P/k_r^2} - 1)\right] \approx \frac{(1 + (a_1 + ib_1)P)(1 + (a_2 + ib_2)P)}{(1 + (a_1 - ib_1)P)(1 + (a_2 - ib_2)P)} \ , \tag{14.36}$$

and require that values a_i, b_i are real. If we further constrain the solution such that all b_i are equal, their common value turns out to be fixed by the first-order term in the expansion. In this case, $b_1 = b_2 = 1/8$, and from the second-order term we find that the $a_1 + a_2 = 1/2$. It also turns out that satisfying the imaginary part of the constraint in lower orders results in satisfying real part of the constrain in the given order. Order three, in this case, then will fix both $a_{1,2}$:

$$a_1 = \frac{1}{4} + \frac{\sqrt{12 + k_r^2 \Delta z^2}}{8\sqrt{3}} \quad , \quad a_2 = \frac{1}{4} - \frac{\sqrt{12 + k_r^2 \Delta z^2}}{8\sqrt{3}} \quad , b_1 = b_2 = \frac{1}{8} \ . \tag{14.37}$$

For this solution the achieved accuracy is such that

$$\exp\left[ik_r \Delta z(\sqrt{1 + P/k_r^2} - 1)\right] = \frac{(1 + (a_1 + ib_1)P)(1 + (a_2 + ib_2)P)}{(1 + (a_1 - ib_1)P)(1 + (a_2 - ib_2)P)} + \frac{i}{128}(k_r \Delta z)(P/k_r^2)^4$$

$$+ \frac{i[270(k_r\Delta z) - 90i(k_r\Delta z)^2 + 15(k_r\Delta z)^3 + (k_r\Delta z)^5]}{23040}(P/k_r^2)^5 + O(P^6) \ . \tag{14.38}$$

Thus, with only three degrees of freedom, and two sub-steps of C-N type one can construct an update scheme that goes two orders beyond the paraxial approximation. This schemes models accurately waves that propagate at 35 degree angle with respect to the axis.

Exercise: Consider approximate evolution operator with $b_1 = b_2 = b_3$ and free a_1, a_2, and a_3. By comparing Taylor expansion of the approximant and of the exact expression, obtain system of equations to determine these coefficients.

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Exercise: Consider approximate evolution operator with $a_1 = a_2 = a_3$. Show that such a solution does not exist.
