Final Project: Nonlinear PDEs in Optics and Second Harmonic Generatoin

Ivan F. Valerio
Department of Physics, Astronomy, and Applied Physics,
Rensselaer Polytechnic Institute
valeri@rpi.edu

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Algorithmic Considerations

For a long time now we have dealt with light traveling in a medium as a linear phenomena. Linearity means that certain properties of the wave's path are independent of the intensity of the light itself. These properties include:

1. The refractive index of the material and absorption coefficient are independent of the light intensity.

2. The principle of superposition holds.

3. The frequency of light itself is not altered.

4. Light does not interact with light inside the medium. They simply superimpose.

But unfortunately we have discovered that this is not an accurate representation of light in a medium. At high enough intensities, the characteristics described above do not hold completely, and new phenomena begin to arise. Tools such as creating a light with a completely new frequency from the interaction of two waves of given frequencies has been recorded, and is widely used in research. Self-focused light is another result of such of non-linear optics in action. Here we will explore a phenomena called Second Harmonic Generation (SHG). This occurs when a light of a certain frequency, with high enough amplitude, produces a second wave with a different frequency.

The equation that describes the motion of a wave in a medium can be derived from Maxwell's equations and are used in many fields. For an arbitrary homogeneous dielectric medium, the differential equation is given by:

$$\nabla^2 E - \frac{1}{c^2}\frac{\partial^2 E}{\partial t^2} = \mu_o \frac{\partial^2 P_{NL}}{\partial t^2} \tag{1}$$

$$P_{NL} = 2dE^2 + 4\chi^{(3)}E^3 + \cdots \tag{2}$$

where c is the speed of the wave in the medium, μ_o is the magnetic permeability of free space, and P_{NL} is the polarization density of the material. The terms of the polarization density arise from the manual taylor expansion performed on it. The reasoning behind it is that typically materials behave linearly at relatively low intenisities, and the nonlinear effects begin to take hold once the intensities increase. The taylor expansion allows us to add these terms as we see fit depending on the intensities. If the intensity is really small, than then polarization density expansion becomes zero, and we have our usual linear partial differential equation of a wave. The terms d and $\chi^{(3)}$ are simply constants determined from the material.

Now here we will only concentrate on the first term in the nonlinear regime. But what does the differential equation represent? The term on the other side of the equal sign in equation (1) can be interepreted as the light producing a polarizatoin density, which in turn *radiates* a field. These fields then continue to interact with each other and as a result we have coupled wave equations.

Further study of this problem can be done by analyzing the discretization of the differential equation.

It is important to note that for a wave to interact with another constructively, the waves have to fulfill the following condition:

$$w_1 + w_2 = w_3 \tag{3}$$

If this condition is not met, then the waves will not interact constructively. Here of course we are only considering three waves of given frequencies. If we are to include a fourth wave, then the condition changes to:

$$w_1 + w_2 = w_3 + w_4 \tag{4}$$

Implementation

Let us now find a discretized form of the wave equation in a nonlinear medium. We know the approximations neccessary for second derivatives in space and time:

$$\frac{\partial^2 E}{\partial x^2} \approx \frac{E_{i+1,j} + E_{i-1,j} - 2E_{i,j}}{(\Delta x)^2} \tag{5}$$

$$\frac{\partial^2 E}{\partial t^2} \approx \frac{E_{i,j+1} + E_{i,j-1} - 2E_{i,j}}{(\Delta t)^2} \tag{6}$$

Where the subsripts i and j represent variables of space and time, respectively. Care must be taken when discretizing the polarization density portion of this equation:

$$\frac{\partial^2 (E^2)}{\partial t^2} \approx \frac{(E_{i,j+1})^2 + (E_{i,j-1})^2 - 2(E_{i,j})^2}{(\Delta t)^2} \tag{7}$$

Now to proceed, we want to observe the individual waves moving along the medium with their respective frequencies. This can be done if we think of the incident wave as a composition of three waves:

$$E(t) = E^{(1)}(t) + E^{(2)}(t) + E^{(3)}(t) \tag{8}$$

If we were to apply this equivalency into the differential equations, and solve for $E_{i,j+1}$, then we would get a system of three equations with cross terms. Here is one of them:

$$\begin{aligned} E^{(1)}_{i,j+1} = \frac{E^{(1)}_{i+1,j} + E^{(1)}_{i-1,j} - 2E^{(1)}_{i,j}}{c'^2/c^2} - 2d\mu_o c^2 \Bigg(&(E^{(1)}_{i,j+1})^2 + E^{(2)}_{i,j+1}E^{(3)}_{i,j+1} + \\ &(E^{(1)}_{i,j-1})^2 + E^{(2)}_{i,j-1}E^{(3)}_{i,j-1} - 2(E^{(1)}_{i,j})^2 - 2E^{(2)}_{i,j}E^{(3)}_{i,j} \Bigg) \\ &-E^{(1)}_{i,j-1} + 2E^{(1)}_{i,j} \end{aligned} \tag{9}$$

A similar equation is implemented for the other superpositions of the electric field. Each of the equations that describe a wave have components of the other waves in them, so as long as there are two waves traveling in the mediumm, there will be a third wave produced, and this wave will have a different frequency to the incident waves. It is important to understand that it is not possible to simply plug in the values and the solution. If we look at equation (9) we see that it has a $(E^{(1)}_{i,j+1})^2$ term on the other side of the equation. This means that we must perform iterations of the equation to obtain an accurate result. In other words, once we obtain $E^{(1)}_{i,j+1}$ we must plug it back into the equation. This iteration is called the first Born approximation. Additional iterations would result on higher orders of Born approximation. Now that we have a form for the coupled equations, we can individually analyze how they evolve as they travel inside the medium.

Results

The following image is the result obtained when a wave travels inside a nonlinear medium:

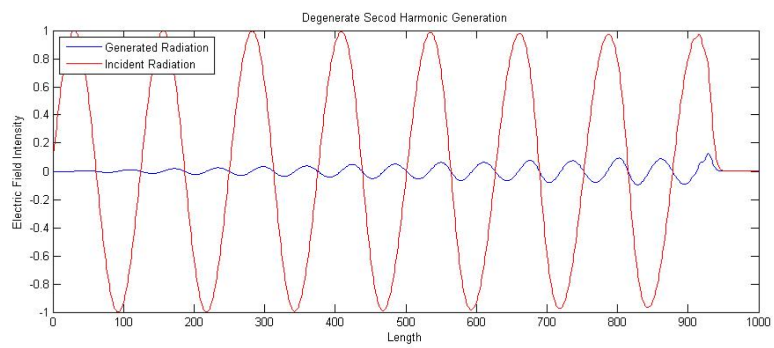

Figure 1: Here we see the intensities of both waves as they move along the medium. The blue curve represents the induced radiation, while the red curve is the incident radiation. While not very accurate at the very end due to the presence of a discontinuity (the program suddenly turns on the wave when there is no field inside the medium, which is in fact an impossibility realistically), the simulation seems to show an accurate picture of what would happen. We can see that as the wave's intensity decreases, the induced wave's intensity increases proportionally. The frequencies are $2w_1 = 2w_2 = w_3$.

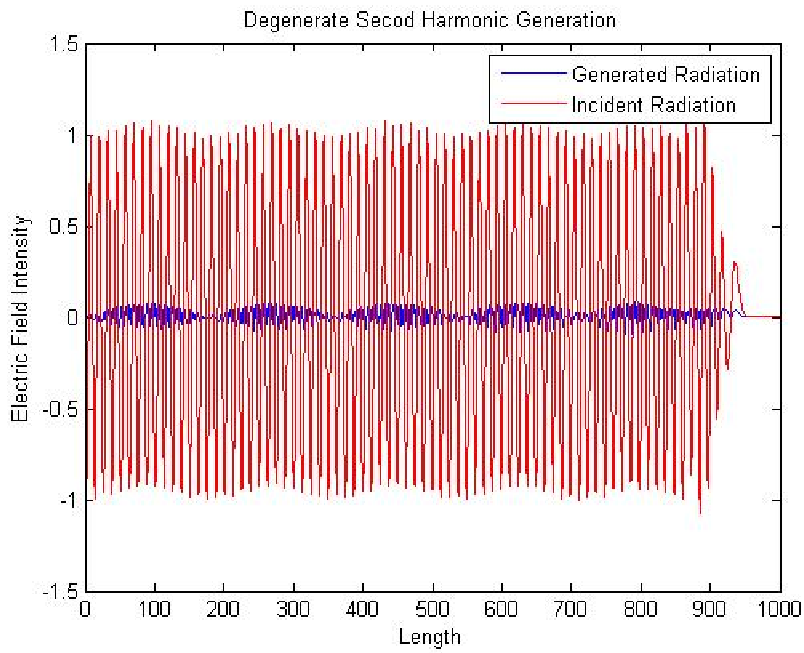

Figure 2: These graph shows a simulation of two waves with the same intensities as the previous waves, but their frequencies are increased 10 fold. We observe something quite interesting: The waves seem to interact more strongly. As the indiuced wave reaches a certain intensity, it too begins to induce a wave. Because of the presence of the other wave, this interaction does not produce a higher frequency, but rather a lower one. This sort of effect is very similar to what is called a down converter in optics, where a higher frequency wave induced a lower frequency wave. Not only that, but the energy between the waves seems to oscillate back and forth, inducing a change in intensity between the two.

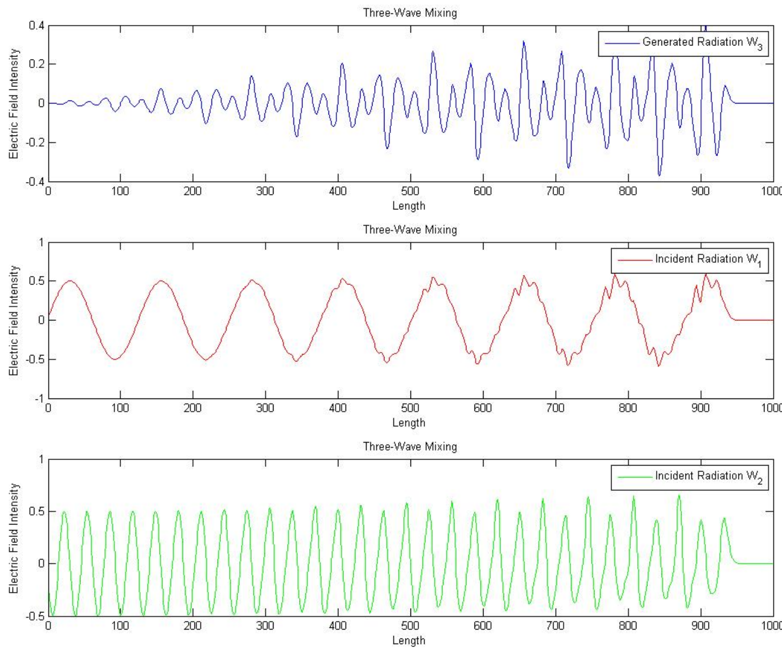

Figure 3: Now we include waves of two different frequencies into the simulation. Above is the image of the results. We begin to see some jitter in the intensities, but this one might think this is due to the discontinuity at the very end of the wave. Later we find that this is actually a fourth frequency being introduced into the wave. Also we see that waves 1 and 2 begin to shift upward. This can be explained by the fact that nonlinear optics can also generate electric fields of zero frequency inside the medium(sometihng similar to Pockel's effect).

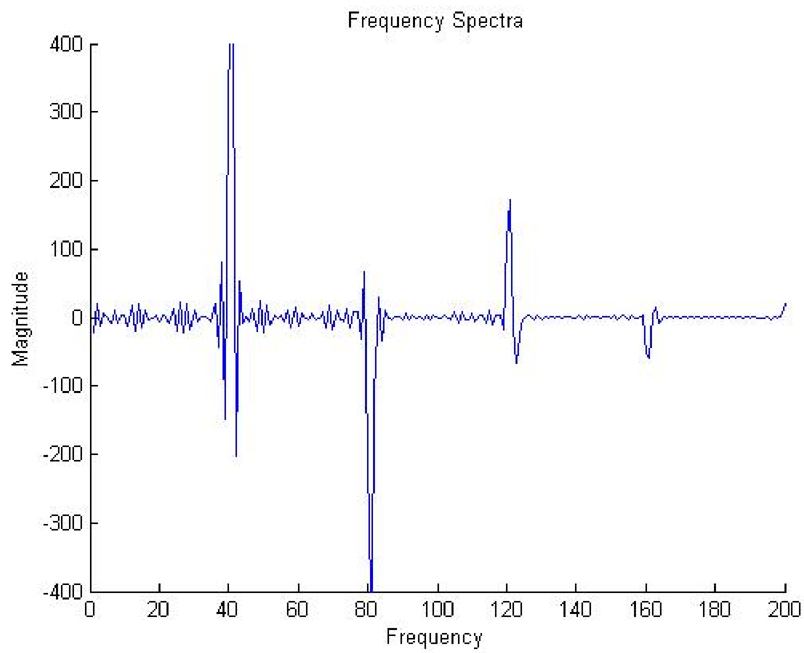

Figure 4: Here is a frequency representation of all the waves put together at a future time. This would be in essence the total electric field inside the medium as all the waves travel together. We can see that there are not only three, but four distinct peaks. Can these peaks be originating from the creation of higher frequencies?It is possible that because we are only modeling three waves, the frequency from a fourth possible wave is leaking into one of the waves. If this were to be animated with time, we would observe an increase in these peaks over time. Also note the distances between the peaks, which represents the conditions we placed earlier about one frequency being the sum or difference of two other frequencies.

Discussion

The effects observed here seem to show effects predicted in optics for simple situations such as second harmonic generation and simple three-wave mixing. Unfortunately, like most computer simulations, this program has its drawbacks. The creation of the wave has the difficulty that it cannot interact too much with the wall at the other end of the medium. Simulation of a "transparent" wall cannot be done when the wave itself has a discontinuity. When this discontinuity reaches the end of the matrix where the data is stored, the boundary condition overcompensates for this sudden change, and as a result the discontinuity is bounced back, destroying the integrity of the wave. This discontinuity then proceeds to propagate back and forth, despite the boundary condition reaching stable operation at both ends.

Another innaccuracy is the presence of small peaks within the larger peaks of the incident wave. Where could these anomalies come from? It is important to understand that the production of a light of a certain frequency will not be specific to one wave vector in the program. The waves are free to interact as they see fit, and frequencies might not be limited to one wave. These "peaks" might just be compoentes of higher frequencies appearing at different places. In this sense we can't limit or prevent this from happening. Further work on this is necessary.

This method can be extended to simulate more than three waves. Although possible, it can be tedious to program, and one must be detail oriented to avoid any programing issues. It would be much easier to simply oserve the evolution of the sum of all the waves. This can have the advantage that it is very straightforward to implement, but it's disadvantage is the inability to obseve individual frequencies. If one were to create such program and then wished to analyze the frequencies, then it would be wise to take the fourier transform of the data, as this will allow one to locate the main frequencies at play in the wave.

Higher order effects are also possible. Earlier we had expanded the polarization density with taylor expansion, and had only applied the second order nonlinear term. Other effects arise when implementing the third order nonlinear term. Granted this would require considerable more work, it would be interesting to see the effects of higher order nonlinear phenomena in light.