Diffraction calculation with FFTs

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April 17, 2017

1 Defining the Integral

This derivation follows what is given by Goodman in "Introduction to Fourier Optics" [1]. We assume that we can describe the Helium beam with a scalar potential which obeys the wave equation,

$$\nabla^2\psi - \frac{1}{\nu^2}\frac{\partial^2\psi}{\partial t^2} = 0. \tag{1}$$

If then also assume that the problem is time independent, we can write ψ as

$$\psi(\vec{r},t) = U(\vec{r})e^{-i\omega t}, \tag{2}$$

meaning that if we set $k = \frac{\omega}{\nu}$, the wave equation can be recast into the Helmholtz equation,

$$(\nabla^2 + k^2)U = 0. \tag{3}$$

In order to proceed further, we will need to use Green's Theorem in the form stated below,

$$\int\int\int_V (U\nabla^2 G - G\nabla^2 U)dv = \int\int_S (U\frac{\partial G}{\partial n} - G\frac{\partial U}{\partial n})ds. \tag{4}$$

G is an arbitrary auxiliary function, however only a good choice of G will lead to solving the diffraction problem. We choose G as a Green's function for the problem so that it satisfies,

$$(\nabla^2 + k^2)G = \delta(\vec{r} - \vec{r_p}) \tag{5}$$

We do need to be careful though, since G is discontinuous at $\vec{r_p}$. So let us break the volume down into two parts, V_ϵ and V' where V_ϵ is a sphere of radius ϵ that surrounds the discontinuity and V' is the rest of the volume we wish to integrate over.

Substitution of equations 3 and 5 into Green's Theorem and performing the integral over V' gives us

$$\int\int\int_V (U(-k^2G) - G(-k^2U))dv = \int\int_{S'} (U\frac{\partial G}{\partial n} - G\frac{\partial U}{\partial n})ds. \tag{6}$$

$$0 = \int\int_{S'} (U\frac{\partial G}{\partial n} - G\frac{\partial U}{\partial n})ds. \tag{7}$$

Where S' is the surface of the volume V' and is made from two parts, the outside surface around the volume enclosing the discontinuity S_ϵ and the outside surface of the whole volume S so that $S' = S + S_\epsilon$. Note that the outward normal from this surface is actual towards $\vec{r_p}$ on S_ϵ. We therefore find that

$$-\int\int_{S_\epsilon} (U\frac{\partial G}{\partial n} - G\frac{\partial U}{\partial n})ds. = \int\int_S (U\frac{\partial G}{\partial n} - G\frac{\partial U}{\partial n})ds. \tag{8}$$

We can compute the left hand side by substituting $G = \frac{\exp{(ik\epsilon)}}{4\pi\epsilon}$ and taking the limit as ϵ goes to zero. Note that the green's function will always take this form when very close to the discontinuity, whatever the boundary conditions. We therefore arrive at the key equation,

$$U(\vec{r_p}) = \int\int_{S_1} (U\frac{\partial G}{\partial n} - G\frac{\partial U}{\partial n})ds \tag{9}$$

Where S_1 is the surface just behind the diffracting screen, the other surface S_2 has been ignored since the wave must obey the Sommerfeld radiation condition [1]. We now make two assumptions to continue, the first is that at the aperture U and $\frac{\partial U}{\partial n}$ are exactly as they would be without the aperture screen being present. The second assumption is that in the plane immediately behind the screen, the integrand is identically zero in the geometric shadow of the aperture. With these assumptions we can then write,

$$U(\vec{r_p}) = \int\int_{\Sigma} (U\frac{\partial G}{\partial n} - G\frac{\partial U}{\partial n})ds \tag{10}$$

Where the integral is now over the plane in the aperture which is open Σ, and U is the amplitude of the scalar field due to the source with no disturbance caused by the aperture.

Kirchoff imposed the second condition described above by setting both U and $\frac{\partial U}{\partial n}$ to zero. However setting both to zero will lead to mathematical inconsistencies, so instead we look for a Green's function which has either G or $\frac{\partial G}{\partial n}$ equal to zero so that we can loosen this very tight criteria. This can be achieved by using the method of images and writing down the function

$$G_{-} = \frac{\exp{(ikr)}}{4\pi r} - \frac{\exp{(ik\tilde{r})}}{4\pi\tilde{r}} \tag{11}$$

Where $r^2 = (x - x_p)^2 + (y - y_p)^2 + (z - L)^2$, $\tilde{r}^2 = (x - \tilde{x}_p)^2 + (y - \tilde{y}_p)^2 + (z + L)^2$, (x_p, y_p) is the co-ordinate of the point we wish to evaluate the integral at and $(\tilde{x}_p, \tilde{y}_p)$ is the point the image source is placed.

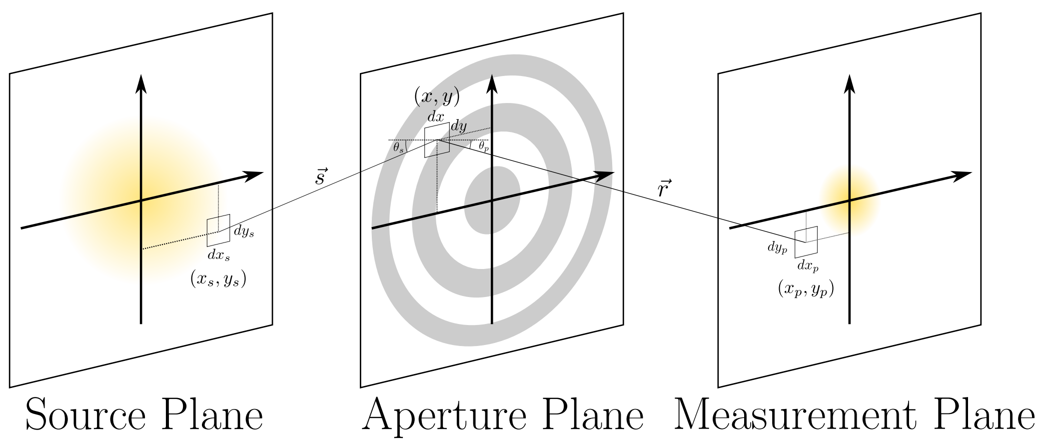

Figure 1: Cartoon of diffraction integral illustrating all of the defined parameters. The source plane is where the source of helium is located, the wave then travels to the zone plate where it is diffracted in the aperture plane. The diffracted intensity is then calculated in the measurement plane.

This choice of Green's function is identically zero in the aperture plane since $r = \tilde{r}$ in the aperture plane. We then set $\frac{\partial U}{\partial n}$ to be zero directly behind the aperture, and the integral now becomes.

$$U_I(\vec{r_p}) = -\int\int_{\Sigma} U\frac{\partial G_{-}}{\partial n}ds \tag{12}$$

If we evaluate $\frac{\partial G_-}{\partial n}$ we get that:

$$\frac{\partial G_-}{\partial n} = \frac{\partial r}{\partial n}\frac{\partial G_-}{\partial r} + \frac{\partial \tilde{r}}{\partial n}\frac{\partial G_-}{\partial \tilde{r}} \tag{13}$$

$$\left.\frac{\partial r}{\partial n}\right|_{z=0} = \frac{1}{2}\frac{2L}{r} = \cos(\theta_p) \tag{14}$$

$$\frac{\partial G_-}{\partial r} = (ik - \frac{1}{r})\frac{\exp(ikr)}{r} \tag{15}$$

$$\left.\frac{\partial G_-}{\partial n}\right|_{z=0} = 2\cos(\theta_p)(ik - \frac{1}{r})\frac{\exp(ikr)}{r} \tag{16}$$

If we now take the incident field to be a spherical wave so that $U(\vec{r}_{S_1}) = a_p\frac{\exp{(iks)}}{s}$ where $s^2 = D^2 + (x - x_0)^2 + (y - y_0)^2$ and assume that $r \gg \lambda$, then we can obtain a value for the amplitude at a point (x_p, y_p, L) by evaluating

$$U_I(\vec{r}_p) = \frac{a_p}{i\lambda}\int\int h(x,y)\frac{\exp(ik(s+r))}{sr}\cos(\theta_p)dxdy \tag{17}$$

After all of this effort we note that this is the same result that is achieved by considering Huygens principle and using an obliquity factor of $K = -\cos\theta_P = \frac{L}{r}$. Since $r(x - x_p, y - y_p)$ is a function of $(x - x_p)$ and $(y - y_p)$ only and $s(x, y)$ is a function of x and y only, we can rewrite the integral as,

$$U_I(\vec{r}_p) = \int\int\left(\frac{a_p}{i\lambda}h(x,y)\frac{\exp(iks(x,y))}{s(x,y)}\right)\left(\frac{\exp(ikr(x-x_p,y-y_p))}{r(x-x_p,y-y_p)}\frac{L}{r(x-x_p,y-y_p)}\right)dxdy \tag{18}$$

$$U_I(\vec{r}_p) = \int\int a(x,y)b(x-x_p,y-y_p)dxdy \tag{19}$$

Where we have defined

$$a(x,y) = \frac{-i}{\lambda}h(x,y)\frac{a_p\exp(iks(x,y))}{s(x,y)} \tag{20}$$

$$b(x-x_p,y-y_p) = \frac{L\exp(ikr(x-x_p,y-y_p))}{r(x-x_p,y-y_p)^2} \tag{21}$$

In this form it becomes clear that this integral is in fact a convolution.

2 Extended Sources and Non-Monochromatic Sources

We can model an extended incoherent source as a sum of point sources. Since the source is incoherent, these imaginary point sources are all incoherent with each other. Therefore, we can find the total intensity by adding up the intensities produced by each point source so we obtain

$$U^{tot}(\vec{r}_p) = \int_{Source} I(\vec{r_S})\left(\int\int a(x,y)b(x-x_p,y-y_p)dxdy\right)d\vec{r_S} \tag{22}$$

Where the extra integral added is over the entire source, $\vec{r_S}$ is a point on the source and $I(\vec{r_S})$ is the intensity distribution of the source.

A similar procedure can be performed to obtain the effect of non-monochromatic beams. Another similar integral is added making the full integral 5 dimensional. Clearly this is now a very complex calculation, however it is normal possible to make a few simplifying assumptions reducing the dimensionality of the calculation. It should be noted that the core of this integral is still a convolution, but it is wrapped in several other integrals and just needs to be calculated many times.

3 Moving to a Discrete System

Since we cannot analytically evaluate this integral we need to numerically evaluate it and this involves using a discrete set of points. We can show that the convolution theorem applies in the discrete case, but it assumes that the convolution is in fact a circular convolution. This means that the matrices involved will need to have cyclic boundary conditions and some care needs to be taken to ensure that the answer is accurate.

We begin by computing the matrix $\mathbf{a}$ over a N_a x N_a grid using a pixel width of Δ, and then computing the matrix $\mathbf{b}$ over a N_b x N_b grid with the same pixel width of Δ. We then zero-pad each of these matrices to be $(N_a + N_b - 1)$ x $(N_a + N_b - 1)$ grids, called $\mathbf{A}$ and $\mathbf{B}$, where we choose Δ in such a way that $(N_a + N_b - 1) = 2^n$ where n is an integer so that the FFT routines later are quick.

We then Fast Fourier Transform (FFT) $\mathbf{A}$ and $\mathbf{B}$ to obtain $\tilde{\mathbf{A}}$ and $\tilde{\mathbf{B}}$ respectively. As the convolution theorem dictates, we then multiply these matrices elementwise to obtain,

$$\tilde{\mathbf{K}} = \tilde{\mathbf{A}} \odot \tilde{\mathbf{B}} \tag{23}$$

The final step is to then Inverse Fast Fourier Transform (IFFT) back to obtain $\mathbf{K}$. From our zero padding earlier, we expect that the central $|N_a - N_b|$ x $|N_a - N_b|$ grid is our best estimate for $\mathbf{U}$ the actual diffraction pattern on the grid we have defined.

References

[1] Joseph W. Goodman. *Introduction to Fourier Optics*. Roberts & Company Publishers, Englewood, Colo, 3rd revised edition edition edition, January 2005.