Grating effect on phase

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We prove that the phase shift caused by a z shift of a grating, or in general any scattering/refracting/diffracting structure, is proportional to the cosine and not 1/cosine. This is done both from the point of view of the "physical optics approximation" which uses scalar diffraction and from the point of view of a full solution to Maxwells Equations. In both cases we work in 2D which is sufficient to show the desired result while signficantly simplifying the analysis. It should be noted that for the encoder, the grating periodicity will only be about twice the wavelength which means the "physical optics approximation", which Goodman uses throughout his book on Fourier Optics, is NOT valid. But the fact that the phase shift is proportional to the cosine is totally independent of the ratio of the wavelength to the grating periodicity. This the reason for showing that exactly the same cosine phase shift occurs in the "physical optics approximation" and in the full Maxwell solution.

I. GENERAL SOLUTIONS

General solutions to the Helmholtz equation for monochromatic light

$$\left(\partial_x^2 + \partial_z^2 + k^2\right) \phi(x, z) = 0$$

which are propagating generically in the $+z$ direction are given by

$$\phi(x, z) = \int d\beta \tilde{\phi}(\beta) \exp\left[i\beta x + i\gamma(\beta) z\right]$$

where

$$\gamma(\beta) = \sqrt{k^2 - \beta^2}$$

with $k = 2\pi/\lambda$ with λ the wavelength. β is the spatial frequency in the x direction, $\gamma(\beta)$ is the spatial frequency in the z direction and

$$\tilde{\phi}(\beta) = \frac{1}{2\pi} \int dx \phi(x, z = 0) \exp\left[-i\beta x\right]$$

is the Fourier transform of $\phi(x, z = 0)$.

To get a general solution propagating generically in the $-z$ direction replace $\exp\left[+i\gamma(\beta) z\right]$ with $\exp\left[-i\gamma(\beta) z\right]$. Given the forms of the upward $(+z)$ propagating and downward $(-z)$ propagating fields we have the following result. The Fourier transform of an upwardly $(+z)$ propagating field at $z \neq 0$ is given by

$$\frac{1}{2\pi} \int dx \phi(x, z) \exp\left[-i\beta x\right] = \exp\left[i\gamma(\beta) z\right] \tilde{\phi}(\beta)$$

That is, the Fourier transform of an upwardly propagating field picks up the phase factor $\exp\left[i\gamma(\beta) z\right]$ relative to the $z = 0$ Fourier transform of the field, $\tilde{\phi}(\beta)$. For z positive, $\gamma(\beta) z$ is positive and for z negative, $\gamma(\beta) z$ is negative. For a downward propagating field the phase factor the Fourier transform picks up relative to the $z = 0$ Fourier transform of the field is $\exp\left[-i\gamma(\beta) z\right]$ and for z positive $-\gamma(\beta) z$ is negative and for z negative $-\gamma(\beta) z$ is positive. Hence in both cases the phase increases in the direction of propagation and decreases in the direction opposite to the direction of propagation.

NOTE: As has been pointed out by many people including the late Doug Goodman (IBM Optics Expert not the Fourier Optics Goodman), one should always work with β and $\gamma(\beta)$ and only in the very end replace these variables with their angle equivalents

$$\beta = k \sin(\theta)$$

$$\gamma(\beta) = \sqrt{k^2 - \beta^2} = k\sqrt{1 - \sin(\theta)^2} = k \cos(\theta)$$

where $\theta =$ the angle measured from the z axis.

II. DIFFRACTION FROM A GRATING

Consider a grating with period P where $P \gg \lambda$ and the depth D of the grating grooves as a function of $x, h(x)$, satisfies $D = \max[h(x)] - \min[h(x)] \ll \lambda$. The reason for choosing $P \gg \lambda$ and $D \ll \lambda$ is that, in this regime, for θ not too large, we can use the physical optics approximation for the effect that the grating has on an incident field in reflection which is simply to multiply the incident field, $\phi_{in}(x,z)$, by the phase factor $\exp[i2kh(x)]$ to get the outgoing or reflected field $\phi_{out}(x,z)$, that is,

$$\phi_{out}(x,z) = \exp[i2kh(x)]\,\phi_{in}(x,z)$$

Here $\phi_{in}(x,z)$ is incident on the grating from below and so z corresponds to a plane infinitesimally below the grating, i.e, $z = \min[h(x)]$.

NOTE: The change in phase caused by shifting the grating is completely independent of the relative sizes of P, λ and D. If we did not assume $P \gg \lambda$ and $D \ll \lambda$ then we would have to solve Maxwells equations with appropriate boundary conditions and we could not treat the effect of the grating as simply multiplying the incident field by the phase factor $\exp[i2kh(x)]$. The same phase effect will be derived below as an exact solution to Maxwell's equations in 2D using the scattering matrix. It is only in the regime where $P \gg \lambda$ and $D \ll \lambda$ that the Maxwell equation solution reduces to just multiplication by the phase factor $\exp[i2kh(x)]$. Any time you treat a grating or any other optical component by simply multiplying by a phase factor you are by definition working in the regime where the surface is slowly varying compare to the wavelength and boundary conditions can be ignored. This is known as the "physical optics approximation". All of Goodman's Fourier Optics book works in the physical optics approximation.

Here's a quote from Goodmans book on Fourier Optics (last paragraph of section 3.2)

> With these discussions as background, we turn away from the vector theory of diffraction to the simpler scalar theory. We close with one final observation. Circuit theory is based on the approximation that circuit elements (resistors, capacitors, and inductors) are small compared to the wavelength of the fields that appear within them, and for this reason can be treated as lumped elements with simple properties. We need not use Maxwell's equations to analyze such elements under these conditions. In a similar vein, the scalar theory of diffraction introduces substantial simplifications compared with a full vectorial theory. The scalar theory is accurate provided that the diffracting structures are large compared with the wavelength of light. Thus the approximation implicit in the scalar theory should be no more disturbing than the approximation used in lumped circuit theory. In both cases it is possible to find situations in which the approximation breaks down, but as long as the simpler theories are used only in cases for which they are expected to be valid, the losses of accuracy will be small and the gain of simplicity will be large.

Since $h(x)$ represents a grating, $h(x)$ is periodic in x, i.e.,

$$h(x) = h(x+P) \;\; \forall x$$

Hence $\exp[i2kh(x)]$ is also periodic with period P as well and can be expressed as a Fourier series

$$\begin{aligned}\exp[i2kh(x)] &= \int d\beta a(\beta)\exp[i\beta x]\sum_n \delta\left(\beta - n\frac{2\pi}{P}\right)\\ &= \sum_n a(n2\pi/P)\exp[in2\pi/Px]\\ &\equiv \sum_n a_n \exp[in\beta_G x]\end{aligned}$$

Here $\delta(\cdots)$ is the Dirac delta function and

$$a(\beta) = \frac{1}{P}\int_{-P/2}^{+P/2} dx \exp[i2kh(x) - i\beta x]$$

NOTE: The important fact in the derivation below is that $h(x)$ is periodic with period P so that $\exp[i2kh(x)]$ is also periodic with period P. We could simply say the effect of the grating on $\phi_{in}(x,z)$ is to multiply it by a phase factor $\exp[i\psi(x)]$ where $\psi(x)$ is periodic with period P. Writing $\psi(x) = 2kh(x)$ just relates $\psi(x)$ to the shape and depth of the grating grooves $h(x)$. This is not necessary, only the periodicity counts in the derivation below.

III. INCIDENT FIELD

Let $\tilde{\phi}(\beta) \to \tilde{\phi}_{in}(\beta - \beta_0)$ with $\tilde{\phi}_{in}(\beta - \beta_0)$ being tightly peaked around β_0 so that $\tilde{\phi}_{in}(\beta - \beta_0)$ drops rapidly to zero for $|\beta - \beta_0| < 2\pi/P \equiv \beta_G$, in which case the width of $\phi_{in}(x,z)$ in the x direction is much larger than P so that it covers many periods of the grating. In other words the incident beam is very collimated.

IV. UNSHIFTED GRATING

Consider first the case where the grating is just infinitesimally above the $z = 0$ plane which we will treat as the unshifted case.

As above, define

$$\beta_G = \frac{2\pi}{P}$$

and set

$$\beta_0 = -\beta_G$$

so that $\phi_{in}(x,z)$ is a beam propagating in the plus z direction and tilted to the left of the $+z$ axis by angle θ_{in} where $\beta_G = k\sin(\theta_{in})$. This angle corresponds to the angle the reflected/diffracted +1 order has going toward the corner cube/retroreflector after the beam at normal incidence reflects/diffracts from the grating. This is exactly the angle of the beam returning to the grating after being reflected from the corner cube/retroreflector.

Using the above results the complex amplitude of the 0 order beam diffracted, in reflection, from the grating is given by

$$\begin{aligned}
\tilde{\phi}_{out}(0) &= \int \frac{dx}{2\pi} \phi_{out}(x,0) \\
&= \int \frac{dx}{2\pi} \exp[i2kh(x)]\,\phi_{in}(x,0) \\
&= \int \frac{dx}{2\pi} \sum_n a_n \exp[in\beta_G x] \int d\beta \tilde{\phi}_{in}(\beta + \beta_G) \exp[i\beta x] \\
&= \sum_n a_n \int d\beta \tilde{\phi}_{in}(\beta + \beta_G) \int \frac{dx}{2\pi} \exp[i(\beta + n\beta_G)x] \\
&= \sum_n a_n \int d\beta \tilde{\phi}_{in}(\beta + \beta_G)\,\delta(\beta + n\beta_G) \\
&= \sum_n a_n \tilde{\phi}_{in}(-n\beta_G + \beta_G) \\
&= a_1 \tilde{\phi}_{in}(0)
\end{aligned}$$

where the last line follows from the fact that $\tilde{\phi}_{in}(\beta - \beta_0) = \tilde{\phi}(\beta + \beta_G)$ is narrowly peaked around $\beta_0 = -\beta_G$ so that $\tilde{\phi}_{in}((1-n)\beta_G)$ is nonzero only for $n = 1$.

V. SHIFTED GRATING

Now consider what happens if the grating is shifted along the z axis a distance $z > 0$.

First evaluate $\phi_{in}(x,z)$ again by first letting β_0 be arbitrary and at the end set it to $-\beta_G$ as in the unshifted case,

$$\phi_{in}(x,z) = \int d\beta \tilde{\phi}_{in}(\beta-\beta_0)\exp\left[i\beta x + i\gamma(\beta) z\right]$$

$$\text{Let } \beta' = \beta - \beta_0$$

$$\phi_{in}(x,z) = \int d\beta' \tilde{\phi}_{in}(\beta')\exp\left[i(\beta_0+\beta')x + i\gamma(\beta_0+\beta') z\right]$$

$$\text{Drop the prime on the dummy integration variable } \beta'$$

$$\phi_{in}(x,z) = \int d\beta \tilde{\phi}_{in}(\beta)\exp\left[i(\beta_0+\beta)x + i\gamma(\beta_0+\beta) z\right]$$

But again, due to the narrowness of the function $\tilde{\phi}_{in}(\beta)$ only small values of $\beta-\beta_0$ will contribute to the integral, hence we can Taylor expand $\gamma(\beta_0+\beta)$ as

$$\gamma(\beta_0+\beta') = \gamma_0 + \gamma_0'\beta + \frac{1}{2}\gamma_0''\beta^2 + \cdots$$

where

$$\begin{aligned}\gamma_0 &= \gamma(\beta_0)\\ \gamma_0' &= \partial_\beta \gamma(\beta)\big|_{\beta=\beta_0}\\ \gamma_0'' &= \partial_\beta^2 \gamma(\beta)\big|_{\beta=\beta_0}\end{aligned}$$

We now show that the term $\gamma_0'\beta$ causes the beam to shift position along x as it propagates in z. The term $1/2\gamma_0''\beta^2$ and higher order terms will cause the beam to spread diffractively as it propagates. These terms are not needed to show how the grating affects the phase and indeed diffraction spreading in any practical case should be negligible.

First compute $\phi_{in}(x,z)$ keeping just $\gamma(\beta_0+\beta) = \gamma_0 + \gamma_0'\beta$

$$\phi_{in}(x,z) = \exp\left[i\beta_0 x + i\gamma_0 z\right]\int d\beta \tilde{\phi}_{in}(\beta)\exp\left[i(x+\gamma_0' z)\beta\right]$$

The dependence on $x+\gamma_0' z$ indicates the beam shifts in x with propagation in z.

Consider the position of the "center" of the beam by setting

$$x = -\gamma_0' z$$

We have

$$\begin{aligned}\phi_{in}(x=-\gamma_0' z, z) &= \exp\left[i(-\beta_0\gamma_0' + \gamma_0) z\right]\int d\beta \tilde{\phi}_{in}(\beta)\\ &= \exp\left[i(-\beta_0\gamma_0' + \gamma_0) z\right]\phi_{in}(0,0)\end{aligned}$$

and so the phase picked up by the beam "center" $\phi_{in}(0,0)$ as it propagates to position $x=-\gamma_0' z$ and z is

$$(-\beta_0\gamma_0' + \gamma_0) z = k\frac{z}{\cos(\theta_{in})}$$

after using $\gamma(\beta) = \sqrt{k^2-\beta^2}$. This is the expected result for the propagation of the beam.

Now, compute the effect of diffraction from the shifted grating on $\phi_{in}(x,z)$, again setting $\beta_0 = -\beta_G$

$$
\begin{aligned}
\tilde{\phi}_{out}(\beta = 0 \text{ at shifted } z \text{ position}) &= \int \frac{dx}{2\pi} \phi_{out}(x,z) \\
&= \int \frac{dx}{2\pi} \exp[i2kh(x)]\, \phi_{in}(x,z) \\
&= \exp[i\gamma_0 z] \int \frac{dx}{2\pi} \exp[i2kh(x) - i\beta_G x] \int d\beta \tilde{\phi}_{in}(\beta) \exp[i(x + \gamma_0' z)\beta] \\
&= \exp[i\gamma_0 z] \int \frac{dx}{2\pi} \exp[i2kh(x - \gamma_0' z) - i\beta_G (x - \gamma_0' z)] \int d\beta \tilde{\phi}_{in}(\beta) \exp[i\beta x] \\
&= \exp[i\gamma_0 z] \int \frac{dx}{2\pi} \sum_n a_n \exp[in\beta_G (x - \gamma_0' z) - i\beta_G (x - \gamma_0' z)] \int d\beta \tilde{\phi}_{in}(\beta) \exp[i\beta x] \\
&= \exp[i\beta_G \gamma_0' z + i\gamma_0 z] \sum_n a_n \exp[-in\beta_G \gamma_0' z] \int d\beta \tilde{\phi}_{in}(\beta) \int \frac{dx}{2\pi} \exp[i(\beta + (n-1)\beta_G)x] \\
&= \exp[i\beta_G \gamma_0' z + i\gamma_0 z] \sum_n a_n \exp[-in\beta_G \gamma_0' z] \int d\beta \tilde{\phi}_{in}(\beta)\, \delta(\beta - (n-1)\beta_G) \\
&= \exp[i\beta_G \gamma_0' z + i\gamma_0 z] \sum_n a_n \exp[-in\beta_G \gamma_0' z]\, \tilde{\phi}_{in}((n-1)\beta_G) \\
&= \exp[i\beta_G \gamma_0' z - i\beta_G \gamma_0' z + i\gamma_0 z]\, a_1 \tilde{\phi}_{in}(0) \\
&= \exp[i\gamma_0 z]\, a_1 \tilde{\phi}_{in}(0) \\
&= \exp[ik\cos[\theta_{in}]\, z]\, a_1 \tilde{\phi}_{in}(0)
\end{aligned}
$$

Here we have used the fact that, again due to the narrowness of $\tilde{\phi}_{in}(\beta)$ around $\beta = 0$, we have only $n = 1$ contributes to the sum.

Conclusion: Comparing the unshifted result $a_1 \tilde{\phi}_{in}(0)$ for the diffracted beam to the shifted result $\exp[ik\cos[\theta]\, z]\, a_1 \tilde{\phi}_{in}(0)$ for the diffracted beam we see that the effect of shifting the grating in z is to multiply the unshifted result by the phase factor $\exp[ik\cos[\theta]\, z]$.

One final step. We should propagate the field reflected/diffracted from the grating back down to the $z = 0$ plane. This amounts simply to multiplying the reflected/diffracted field by $\exp[ikz]$ and so we have finally

$$\exp[ikz + ik\cos[\theta_{in}]\, z]$$

VI. FULL MAXWELL SOLUTION

In 2D with coordinates x and z if we take the electric field $\vec{E}$ to be purely polarized in the y direction, $\vec{E} = E_y \hat{y}$ then we can set

$$\phi(x,z) = E_y(x,z)$$

and Maxwell's equations, for monochromatic light, reduce to the Helmholtz equation

$$\left(\partial_x^2 + \partial_y^2 + k^2 n(x,z)^2\right)\phi(x,z) = 0$$

where $k = 2\pi/\lambda$ with λ the wavelength in vacuum and $n(x,z)$ is the index of refraction as a function of position x and z.

Consider the case where

$$
\begin{gathered}
n(x,z)^2 = 1 + \Delta n(x,z)^2 \\
\text{with} \\
\Delta n(x,z)^2 \neq 0 \text{ only for } z < 0
\end{gathered}
$$

$$\left(\partial_x^2 + \partial_y^2 + k^2\left(1 + \Delta n(x,z)^2\right)\right)\phi(x,z) = 0$$

So, in the half-space $z > 0$ the index of refraction is 1 everywhere and it only varies from 1 in the half space $z < 0$. The function $\Delta n(x,z)^2$ can represent any type of index distribution: a grating, a lens, a combination of gratings and lenses, a "lump" of "stuff", whatever, that sits in the half space $z < 0$ and scatters/refracts/diffracts light. We will refer to is as a "scattering structure".

Let

$$\phi(x,z) = \phi_{in}(x,z) + \phi_{out}(x,z)$$

Take $\phi_{in}(x,z)$ to have the Fourier form

$$\phi_{in}(x,z) = \int d\beta_{in}\tilde{\phi}_{in}(\beta_{in})\exp[i\beta_{in}x - i\gamma_{in}z]$$

with

$$\gamma_{in} = \gamma(\beta_{in}) = \sqrt{k^2 - \beta_{in}^2}$$

NOTE: In this section we have taken the incident field to be propagating generically in the $-z$ direction, thus the outgoing or scattered field, for $z > 0$, will be propagating generically in the $+z$ direction.

If $\tilde{\phi}_{in}(\beta)$ is a specified function of β then $\phi_{in}(x,z)$ is a specified incoming or incident field propagating in the $-z$ direction and coming effectively from $z = \infty$. From the specified form of $\phi_{in}(x,z)$ we have that $\phi_{in}(x,z)$ satisfies the Helmholtz equation with $\Delta n(x,z)^2 = 0$,

$$\left(\partial_x^2 + \partial_z^2 + k^2\right)\phi_{in}(x,z) = 0$$

Substituting $\phi = \phi_{in} + \phi_{out}$ into the Helmholtz equation and using the above result for $\phi_{in}(x,z)$ the Helmholtz equation becomes

$$\left(\partial_x^2 + \partial_y^2 + k^2\left(1 + \Delta n(x,z)^2\right)\right)\phi_{out}(x,z) = -k^2\Delta n(x,z)^2\phi_{in}(x,z)$$

This has the form of a "scattering equation". Light traveling generically in the $-z$ with the specified amplitude distribution $\phi_{in}(x,z)$ is incident on the "scattering structure" $\Delta n(x,z)^2$ and $\phi_{out}(x,z)$ is the light distribution generated by the "scattering structure" $\Delta n(x,z)^2$.

Since by definition $\Delta n(x, z \geq 0) = 0$ from the "scattering equation" above we have for $z \geq 0$,

$$\left(\partial_x^2 + \partial_y^2 + k^2\right)\phi_{out}(x, z \geq 0) = 0$$

Given this result it follows that $\phi_{out}(x, z \geq 0)$ can be written in the Fourier transform form

$$\phi_{out}(x, z \geq 0) = \int d\beta_{out}\tilde{\phi}_{out}(\beta_{out})\exp[i\beta_{out}x + i\gamma_{out}z]$$

with

$$\gamma_{out} = \gamma(\beta_{out}) = \sqrt{k^2 - \beta_{out}^2}$$

A. The Scattering Matrix

The scattering matrix $S(\beta_{out}, \beta_{in})$ is defined as the matrix that, via matrix multiplication, converts the column vector $\tilde{\phi}_{in}(\beta_{in})$ into the column vector, $\tilde{\phi}_{out}(\beta_{out})$. Since here the values of β_{in} and β_{out} are continuous, matrix multiplication takes the form of an integral rather than a sum, i.e.,

$$\tilde{\phi}_{out}(\beta_{out}) = \int d\beta_{in} S(\beta_{out}, \beta_{in})\tilde{\phi}_{in}(\beta_{in})$$

Assume that by one means or another we have solved Maxwells equations for the scattering structure to get the scattering matrix $S(\beta_{out}, \beta_{in})$.

B. Shifting the Scattering Structure

Now shift the scattering structure, e.g., the grating, by $-\Delta x$ in x and $-\Delta z$ in z by letting

$$\Delta n(x,z)^2 \to \Delta n(x+\Delta x, z+\Delta z)^2$$

But this is equivalent to leaving the scattering structure unshifted and shifting the incoming and outgoing fields $\phi_{in}(x,z)$ and $\phi_{out}(x,z)$ by $+\Delta x$ and $+\Delta z$. From the Fourier representations for $\phi_{in}(x,z)$ and $\phi_{out}(x,z)$ we have the shifted values of $\tilde{\phi}_{in}(\beta_{in})$ and $\tilde{\phi}_{out}(\beta_{out})$, call them $\tilde{\phi}_{in}^{shifted}(\beta_{in})$ and $\tilde{\phi}_{out}^{shifted}(\beta_{out})$, are given by

$$\begin{aligned}\tilde{\phi}_{in}^{shifted}(\beta_{in}) &= \exp\left[i\beta_{in}\Delta x - i\gamma(\beta_{in})\Delta z\right]\tilde{\phi}_{in}(\beta_{in}) \\ \tilde{\phi}_{out}^{shifted}(\beta_{out}) &= \exp\left[i\beta_{out}\Delta x + i\gamma(\beta_{out})\Delta z\right]\tilde{\phi}_{out}(\beta_{out})\end{aligned}$$

In the formula above for calculating $\tilde{\phi}_{out}(\beta_{out})$ given the scattering matrix $S(\beta_{out},\beta_{in})$ and $\tilde{\phi}_{in}(\beta_{in})$, multiply both sides by

$$\exp\left[i\beta_{out}\Delta x + i\gamma(\beta_{out})\Delta z\right]$$

and multiply $\tilde{\phi}_{in}(\beta_{in})$ by

$$1 = \exp\left[-i\beta_{in}\Delta x + i\gamma(\beta_{in})\Delta z\right]\exp\left[i\beta_{in}\Delta x - i\gamma(\beta_{in})\Delta x\right]$$

to get

$$\begin{aligned}\exp\left[i\beta_{out}\Delta x + i\gamma(\beta_{out})\Delta z\right]\tilde{\phi}_{out}(\beta_{out}) &= \int d\beta_{in}\exp\left[i\beta_{out}\Delta x + i\gamma(\beta_{out})\Delta z\right]S(\beta_{out},\beta_{in})\exp\left[-i\beta_{in}\Delta x + i\gamma(\beta_{in})\Delta z\right] \\ &\quad\times\exp\left[i\beta_{in}\Delta x - i\gamma(\beta_{in})\Delta x\right]\tilde{\phi}_{in}(\beta_{in}) \\ &\text{or} \\ \tilde{\phi}_{out}^{shifted}(\beta_{out}) &= \int d\beta_{in}\exp\left[i\beta_{out}\Delta x + i\gamma(\beta_{out})\Delta z\right]S(\beta_{out},\beta_{in})\exp\left[-i\beta_{in}\Delta x + i\gamma(\beta_{in})\Delta z\right]\tilde{\phi}_{in}^{shiftted}(\end{aligned}$$

From this it follows that the scattering matrix for the shifted scattering structure is given by

$$S^{shifted}(\beta_{out},\beta_{in}) = \exp\left[i(\beta_{out}-\beta_{in})\Delta x + i(\gamma(\beta_{out}) + i\gamma(\beta_{in})\Delta z)\right]S(\beta_{out},\beta_{in})$$

Since

$$\beta = k\sin(\theta)$$

we have

$$\gamma(\beta) = \sqrt{k^2-\beta^2} = k\cos(\theta)$$

and see immediately that shifting scattering structure, i.e, the grating, by Δz adds the phase

$$k\left(\cos(\theta_{out}) + \cos(\theta_{in})\right)\Delta z$$

which is a direct cosine dependence and not 1/cosine.

C. Greens function → Scattering Matrix

For completeness we now show how the Greens function relates to the scattering matrix.
For the Helmholtz equation above, the Greens function $G(x,z,x',z')$ is the function that satisfies

$$\left(\partial_x^2 + \partial_y^2 + k^2\left(1+\Delta n(x,z)^2\right)\right)G(x,z,x',z') = \delta(x-x')\,\delta(z-z')$$

where $\delta(\cdots)$ is a Dirac delta function. Effectively the Greens function is the inverse of the differential operator $\left(\partial_x^2 + \partial_y^2 + k^2\left(1+\Delta n(x,z)^2\right)\right)$. That is, when the differential operator acts on the Greens function it yields the identity matrix which for continuous variables is a Dirac delta function.

With the Greens function the solution for $\phi_{out}(x,z)$ is given by

$$\phi_{out}(x,z) = -k^2 \int dx' dz' G(x,z,x',z') \Delta n(x',z')^2 \phi_{in}(x',z')$$

We are not going to solve explicitly for the Greens function. The explicit form is not necessary to show how the scattering matrix is related to the Greens function. So, assume by one means or other we have solved for the Greens function. Substitute the Fourier transform representations of $\phi_{in}(x,z)$ and $\phi_{out}(x,z)$ into the Greens function solution for $\phi_{out}(x,z)$ for $z \geq 0$ to get

$$\begin{aligned}
&\int d\beta_{out} \tilde{\phi}_{out}(\beta_{out}) \exp[i\beta_{out}x + i\gamma_{out}z] \\
&= -k^2 \int dx' dz' G(x,z,x',z') \int d\beta_{in} \tilde{\phi}_{in}(\beta_{in}) \exp[i\beta_{in}x' - i\gamma_{in}z'] \\
&= \int d\beta_{in} \left(-k^2 \int dx' dz' G(x,z,x',z') \exp[i\beta_{in}x' - i\gamma_{in}z'] \right) \tilde{\phi}_{in}(\beta_{in})
\end{aligned}$$

Set

$$z = 0$$

and inverse Fourier transform both sides to get

$$\tilde{\phi}_{out}(\beta_{out}) = \int d\beta_{in} \left(-k^2 \int \frac{dx}{2\pi} dx' dz' G(x,0,x',z') \exp[i\beta_{in}x' - i\beta_{out}x - i\gamma_{in}z'] \right) \tilde{\phi}_{in}(\beta_{in})$$

Comparing this result with the definition of the scattering matrix above we have

$$S(\beta_{out}, \beta_{in}) = -k^2 \int \frac{dx}{2\pi} dx' dz' G(x,0,x',z') \exp[i\beta_{in}x' - i\beta_{out}x - i\gamma_{in}z']$$

The Greens function for the shifted scattering structure is the shifted Greens function and when that is substituted into the above formula for $S(\beta_{out}, \beta_{in})$ in terms of $G(x,z,x',z')$ we get the same result for the shifted scattering matrix as in the previous section.

D.