Optics equations for diffraction of matter wave: CODE vs PAPER.

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Dr. McMorran's code presents three functions (gp0, gp1 and gp2) that calculate how the electron beam intensity varies as it propagates through gratings (along z-direction). The equations used in these functions come from the paper "Model for partial coherence and wavefront curvature in grating interferometers" by McMorran and Cronin, 2008 (http://journals.aps.org/pra/abstract/10.1103/PhysRevA.78.013601).

The form that some of the equations were written in the code presented in Dr. McMorran's thesis is not the same as they are shown in the paper (some algebra was performed in the code equations). We tried to rewrite the paper equations so they could match the ones in the code; we spotted a few differences. We are not sure if these were algebra mistakes or if we don't fully understand why these terms were needed or not.

In this document we try to show what these differences were, so we can ask Dr. McMorran about it the future.

A few other things about the equations - regarding the Fourier components of gratings' complex tranmission function - are not completely understood yet. This document also tries to make explicit what these misunderstood problems are.

1) Equations at function gp2:

1.1) In the code, $d_1 = d_2$. We have the following equations:

a) "coef" refers to equation (18e) in McMorran, 2008.

```
coef = Exp[-Pi * ((dn * Sin[θ] * λ * z23)/(d2 * el3y))^2] * Exp[-Pi * ((λ * z23 * (dn * Cos[θ] + dm * z13/z23))/(d1 * el3x))^2]
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b) The equation below relates to the argument of equation (18d) in the paper. This is where lots of algebra was performed and it is where we found a few differences.

```
phi =
  (dn * n * (1 - z23/v3x) * Cos[θ]^2 + dn * n * (1 - z23/v3y) * Sin[θ]^2 + dn * m * (1 - z13/v3x) * Cos[θ] +
     dm * n * (1 - z13/v3x) * Cos[θ] + dm * m * z13/z23 * (1 - z13/v3x)) *
   ((2 * π * λ * z23)/d1^2) - (2 * π * dn * G2x)/d2;
```

c) The factor that is being subtracted for "phi" in the equation below refers to the argument of equation (18c) in the paper. However, the argument of (18c) has a term with the variable "y", which we think is set to zero in the code (CONFIRM this with Dr. McMorran).

```
phiX = phi - (2 * π * x)/d2 * (dn * Cos[θ] * (1 - z23/v3x) + dm * (1 - z13/v31x));
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d) The exponential multypling the first term in the equation below refers to equation (18b) in the paper. Here we spot another difference: assuming variable "y" is indeed set to zero as stated above, the exponential in equation (18b) that contains a "y" term is of the form e^{a*y+b} ("a" and "b" constants), unlike the exponential term in equation (18c), which is of the form e^{a*y}. For equation (18b), by setting y=0 a constant term e^{b} would still remain. We suspect this missing term could be the the subtracting $-\frac{2*\pi*dn*G2x}{d_2}$ term in equation (1.1b) above, which we could not understand the origin (see section 1.2 below); however, we're not sure (CONFIRM this with Dr. McMorran).

```
ix = (Re[coef] * Cos[phiX] - Im[coef] * Sin[phiX]) *
   Exp[-π * (((x - (λ * z23/d1) * (n * Cos[θ] + m * z13/z23)))/w3x)^2];
```

1.2) Now, we take the argument of equation (18d) in the paper and try to rewrite so it matches to the equation in (1.1b) above.

a) First, we write equation (18d) below as it is in the paper (ϕ is replaced by θ, rx(z3) replaced by $v_{3\,x}$ and ry(z3) replaced by v3y, so it looks more like the way it is written in the code).

$$P = \mathrm{Exp}\left[\frac{i\, 2\,\pi\,\lambda\, z_{13}\, dm}{d_1} * \left(\frac{n\,\mathrm{Cos}[\theta]}{d_2} + \frac{m}{d_1}\right) * \left(1 - \frac{z_{13}}{v_{3\,x}}\right)\right] * \mathrm{Exp}\left[\frac{i\, 2\,\pi\,\lambda\, z_{23}\, dn}{d_2} * \left(\frac{m\,\mathrm{Cos}[\theta]}{d_1} * \left(1 - \frac{z_{13}}{v_{3\,x}}\right) - \frac{n\, z_{23}}{d_2} * \left(\frac{\mathrm{Cos}[\theta]^2}{v_{3\,x}} + \frac{\mathrm{Sin}[\theta]^2}{v3y}\right)\right)\right];$$

b) By simply summing the argument of the two exponentials above, we simply obtain the following "total" argument:

$$\mathrm{argumentP} = \frac{i\, 2\,\pi\,\lambda\, z_{13}\, dm}{d_1} * \left(\frac{n\,\mathrm{Cos}[\theta]}{d_2} + \frac{m}{d_1}\right) * \left(1 - \frac{z_{13}}{v_{3\,x}}\right) + \frac{i\, 2\,\pi\,\lambda\, z_{23}\, dn}{d_2} * \left(\frac{m\,\mathrm{Cos}[\theta]}{d_1} * \left(1 - \frac{z_{13}}{v_{3\,x}}\right) - \frac{n\, z_{23}}{d_2} * \left(\frac{\mathrm{Cos}[\theta]^2}{v_{3\,x}} + \frac{\mathrm{Sin}[\theta]^2}{v3y}\right)\right);$$

c) Now, we try to pull out of the parenthesis a term $\frac{2*\pi*\lambda*z_{23}}{d_1{}^2}$, just like we have for equation (1.1b) above. We omit the i constant from the argument as in the code. Also, notice that the code uses d_1=d_2.

$$\mathrm{argumentP} = \frac{2*\pi*\lambda*z_{23}}{d_1{}^2} * \left(\frac{z_{13}}{z_{23}}\, dm * (n\,\mathrm{Cos}[\theta] + m) * \left(1 - \frac{z_{13}}{v_{3\,x}}\right) + dn * \left(m\,\mathrm{Cos}[\theta] * \left(1 - \frac{z_{13}}{v_{3\,x}}\right) - n\, z_{23} * \left(\frac{\mathrm{Cos}[\theta]^2}{v_{3\,x}} + \frac{\mathrm{Sin}[\theta]^2}{v3y}\right)\right)\right);$$

d) Now, we rearrange the terms inside the outter parenthesis to make the equation more similar to (1.1b):

$$\mathrm{argumentP} = \frac{2*\pi*\lambda*z_{23}}{d_1{}^2} * \left(\frac{z_{13}}{z_{23}}\, dm\, n \left(1 - \frac{z_{13}}{v_{3\,x}}\right) \mathrm{Cos}[\theta] + \frac{z_{13}}{z_{23}}\, dm\, m \left(1 - \frac{z_{13}}{v_{3\,x}}\right) + dn\, m \left(1 - \frac{z_{13}}{v_{3\,x}}\right) \mathrm{Cos}[\theta] - dn\, n\, z_{23} \left(\frac{\mathrm{Cos}[\theta]^2}{v_{3\,x}} + \frac{\mathrm{Sin}[\theta]^2}{v3y}\right)\right);$$

e) We see a couple of differences here: first, the term $\frac{z_{13}}{z_{23}}\, dm\, n \left(1 - \frac{z_{13}}{v_{3\,x}}\right) \mathrm{Cos}[\theta]$

above has a $\frac{z_{13}}{z_{23}}$ factor, while in (1.1b) it is only $dm * n * \left(1 - \frac{z_{13}}{v_{3x}}\right) * \mathrm{Cos}[\theta]$. Second, the term above with the sines and cosines squared is: $dn\, n\, z_{23}\left(\frac{\mathrm{Cos}[\theta]^2}{v_{3x}} + \frac{\mathrm{Sin}[\theta]^2}{v3y}\right)$. However, in (1.1b) appears as $dn * n * \left(1 - \frac{z_{23}}{v_{3x}}\right) * \mathrm{Cos}[\theta]^2 + dn * n * \left(1 - \frac{z_{23}}{v3y}\right) * \mathrm{Sin}[\theta]^2$, which is equal to

$$\left(dn * n - dn * n * \frac{z_{23}}{v_{3x}}\right) * \mathrm{Cos}[\theta]^2 + \left(dn * n - dn * n * \frac{z_{23}}{v3y}\right) * \mathrm{Sin}[\theta]^2$$

e2) which equals

$$dn * n * \mathrm{Cos}[\theta]^2 - dn * n * \frac{z_{23}}{v_{3x}} \mathrm{Cos}[\theta]^2 + dn * n * \mathrm{Sin}[\theta]^2 - dn * n * \frac{z_{23}}{v3y} * \mathrm{Sin}[\theta]^2$$

e3) which equals (using identity $\mathrm{Sin}^2[\theta] + \mathrm{Cos}^2[\theta] = 1$)

$$dn * n - dn * n * z_{23}\left(\frac{\mathrm{Cos}[\theta]^2}{v_{3x}} + \frac{\mathrm{Sin}[\theta]^2}{v3y}\right)$$

f) The second term above is exactly the same as the last term in (1.2d). (1.2d) does not present the "$+dn * n$" term. Hence, the code seems to be inserting a "$+dn * n$"term and also missing a $\frac{z_{13}}{z_{23}}$ factor as shown in (1.2e).

g) The last difference was already mentioned in (1.1d). The equation for phi has a subtracting term "$\frac{2 * \pi * dn * G2x}{d_2}$" does not seem to arise from the equations in the paper. Is our supposition in (1.1d) correct?

CONFIRM whole section 1.2e with Dr. McMorran!

2) Questions about the phase shift: ReT and ImT versus Sinc

Inside functions gp1 and gp2, we have an IF statement that, according to our understanding, selects if phase shift effects are going to be considered or not in the code. This is the part that we understand the least.

2.1) First, let's start with gp1. We understand that:

a) if there are no phase shift effects, the Fourier coefficients are chosen to be sinc functions (in the paper, these are the a_m, a_n coefficients). Our hypotesis is that this arises from assuming that the transmission function is taken to be a rect(x) function (see http://demonstrations.wolfram.com/RectangularPulseAndItsFourierTransform/), which the Fourier transform is a sinc function. However, the Fourier transform of rect(x-x0) has an extra exponential term, as shown in the link. Therefore, we are not sure if our hypothesis is right because this exponential is missing in the code equations.

b) if there is a phase shift into play, the ReT and ImT arrays are used instead. The coefficients then are said to be ReT + i*ImT. ReT is a cosine(phase_shift) and ImT a sine(phase_shift). Why is that? We don't understand why this arrays are used as the Fourier coefficients and neither why the value these two array receive are cosine and sine of the phase shifts.

2.2) Now, we look at gp2. The same facts mentioned for gp1 also apply here, but there is one extra doubt:

a) in gp2, now we have 4 Fourier coeffcients: a_m, a_n , b_m and b_n. So far so good. However, the IF statement that selects if phase shifts will be accounted for or not only does this for two of the coefficients. The other two coefficients are automatically set to use the ReT / ImT values. Is that right? In this case, wouldn't these two last ones be receiving null values when we don't want to include phase shift effects? We know that we will eventually only want to run the code with the phase shift; however, isn't this inconsistent with the logic of the code?