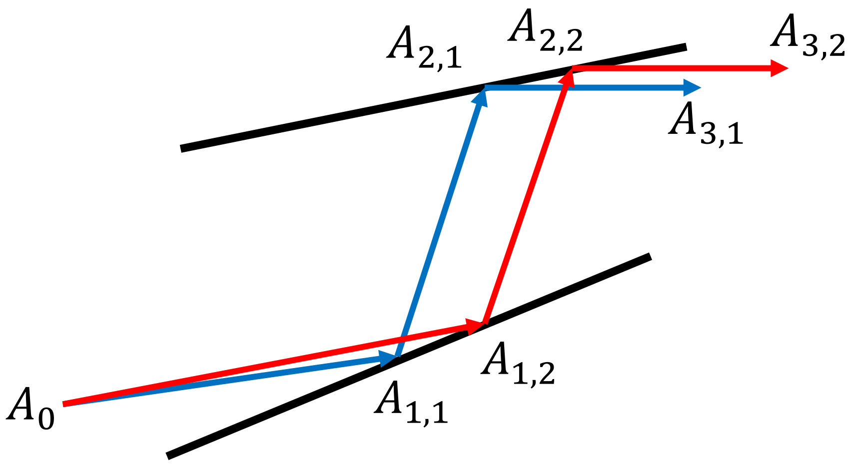
About the validity of the numerical simulation

In the numerical simulation of the dynamical diffraction process, I have used the following methods to calculate the propagation phase. In this note, I try to prove that my treatment is valid.



Assume that the trajectory looks like this one. Here, the red line and blue line correspond to two different monochromatic plane wave.

Assume that from t_0, the blue line (the reference line), and the red line (the novel line) start from position A_0. The amplitude at location A_0 is:

$$red: E_1 e^{i(k_1 r_{A_0} - \omega_1 t_0)}$$

$$blue: E_2 e^{i(k_2 r_{A_0} - \omega_2 t_0)}$$

The reason that we can assume that they start at the same location is that:

1. We are only interested in the propagation phase difference in the end.
2. Plane wave are defined across the whole space. We can always take the value of the two plane wave at the position A_0 at time t_0 and consider this as the starting point the analysis. In this way, we store the initial information to the amplitude of the plane waves.

Now, assume that some time pass by so that:

$$t_{final} = t_0 + \frac{|A_{1,1} - A_0| + |A_{2,1} - A_{1,1}| + |A_{3,1} - A_{2,1}|}{c}$$

Here, c is the speed of light. Then heuristically, we may consider the phase front of the blue line has arrived at the observation point $A_{3,1}$. Then at this new time t_{final}, what the total field of the two plane-waves? Let us analyze this as the following.

The reference wave: The blue wave

We first calculate the wave at position $A_{1,1}$, when the phase front of the blue wave just arrives at this position.

The time interval is:

$$\delta t_{1,1} = \frac{|r_{A_{1,1}} - r_{A_0}|}{c}$$

Therefore, the field is:

$$E_1 e^{i\left(k_1 r_{A_{1,1}} - \omega_1 (t_0 + \delta t_{1,1})\right)}$$

Assume that the reflection can be considered as a simple constant as $R_{1,1}$. Then the reflected field is:

$$R_{1,1} E_1 e^{i\left(k_{1,1}\left(r - r_{A_{1,1}}\right) - \omega_{1,1}(t - t_0 - \delta t_1) + k_1 r_{A_{1,1}} - \omega_1 (t_0 + \delta t_{1,1})\right)}$$

Therefore, at location $A_{2,1}$, at the time when the phase front arrives, the field is:

$$R_{1,1} E_1 e^{i\left(k_{1,1}\left(r_{A_{2,1}} - r_{A_{1,1}}\right) - \omega_{1,1}(t_0 + \delta t_{1,1} + \delta t_{2,1} - t_0 - \delta t_{1,1}) + k_1 r_{A_{1,1}} - \omega_1 (t_0 + \delta t_{1,1})\right)}$$

Here

$$\delta t_{2,1} = \frac{|r_{A_{2,1}} - r_{A_{1,1}}|}{c}$$

Then the reflected pulse is:

$$R_{2,1} R_{1,1} E_1 e^{i\left(k_{2,1}\left(r - r_{A_{2,1}}\right) - \omega_{2,1}(t - t_0 - \delta t_{1,1} - \delta t_{2,1}) + k_{1,1}\left(r_{A_{2,1}} - r_{A_{1,1}}\right) - \omega_{1,1} \delta t_{2,1} + k_1 r_{A_{1,1}} - \omega_1 (t_0 + \delta t_{1,1})\right)}$$

At the final observation position, at the time when the phase front of the blue line arrives, is blue field is:

$$R_{2,1} R_{1,1} E_1 e^{i\left(k_{2,1}\left(r_{A_{3,1}} - r_{A_{2,1}}\right) - \omega_{2,1} \delta t_{3,1} + k_{1,1}\left(r_{A_{2,1}} - r_{A_{1,1}}\right) - \omega_{1,1} \delta t_{2,1} + k_1 r_{A_{1,1}} - \omega_1 (t_0 + \delta t_{1,1})\right)}$$

Notice that:

$$k_{2,1}\left(r_{A_{3,1}} - r_{A_{2,1}}\right) = |k_{2,1}||A_{3,1} - A_{2,1}|$$

$$= c|k_{2,1}| \times \frac{|A_{3,1} - A_{2,1}|}{c} = \omega_{2,1} \delta t_{3,1}$$

Therefore, the field has expression:

$$R_{2,1} R_{1,1} E_1 e^{i(k_1 r_{A_0} - \omega_1 t_0)}$$

The reference wave: The blue wave

Assume that at the time when the phase front of the **blue line** (reference plane wave) arrives at the observation point $A_{3,1}$, the phase front of the **red line** arrives at $A_{3,2}$. Then the same argument shows that the field of the red line at $A_{3,2}$ is:

$$R_{2,2}R_{1,2}E_2e^{i(k_2r_{A_0}-\omega_2t_0)}$$

The general formula of the red line plane wave at this time is:

$$R_{2,2}R_{1,2}E_2e^{i\left(k_{2,2}\left(r-r_{A_{2,2}}\right)-\omega_{2,2}(t_{final}-t_0-\delta t_{1,2}-\delta t_{2,2})+k_{1,2}\left(r_{A_{2,2}}-r_{A_{1,2}}\right)-\omega_{1,2}\delta t_{2,2}+k_2r_{A_{1,2}}-\omega_2(t_0+\delta t_{1,2})\right)}$$

$$= R_{2,2}R_{1,2}E_2e^{i\left(k_{2,2}\left(r-r_{A_{2,2}}\right)-k_{2,2}\left(r_{A_{3,2}}-r_{A_{2,2}}\right)+k_2r_{A_0}-\omega_2t_0\right)}$$

$$= R_{2,2}R_{1,2}E_2e^{i(k_2r_{A_0}-\omega_2t_0)}e^{i\left(k_{2,2}\left(r-r_{A_{3,2}}\right)\right)}$$

Final field

Therefore, the electric field at the final observation point $A_{3,1}$ is:

$$R_{2,1}R_{1,1}E_1e^{i(k_1r_{A_0}-\omega_1t_0)} + R_{2,2}R_{1,2}E_2e^{i(k_2r_{A_0}-\omega_2t_0)}e^{i\left(k_{2,2}\left(r_{A_{3,1}}-r_{A_{3,2}}\right)\right)}$$

$$= R_{2,1}R_{1,1}E_1(t_0,A_0) + R_{2,2}R_{1,2}E_2(t_0,A_0)\exp\left(ik_{2,2}^T\left(r_{A_{3,1}}-r_{A_{3,2}}\right)\right)$$

This is exactly how I have calculated the propagational phase in the numerical dynamical diffraction simulation.

Therefore, there might be unexpected implementation error in the code, the idea itself is exactly the same as the Gaussian approximation theory.