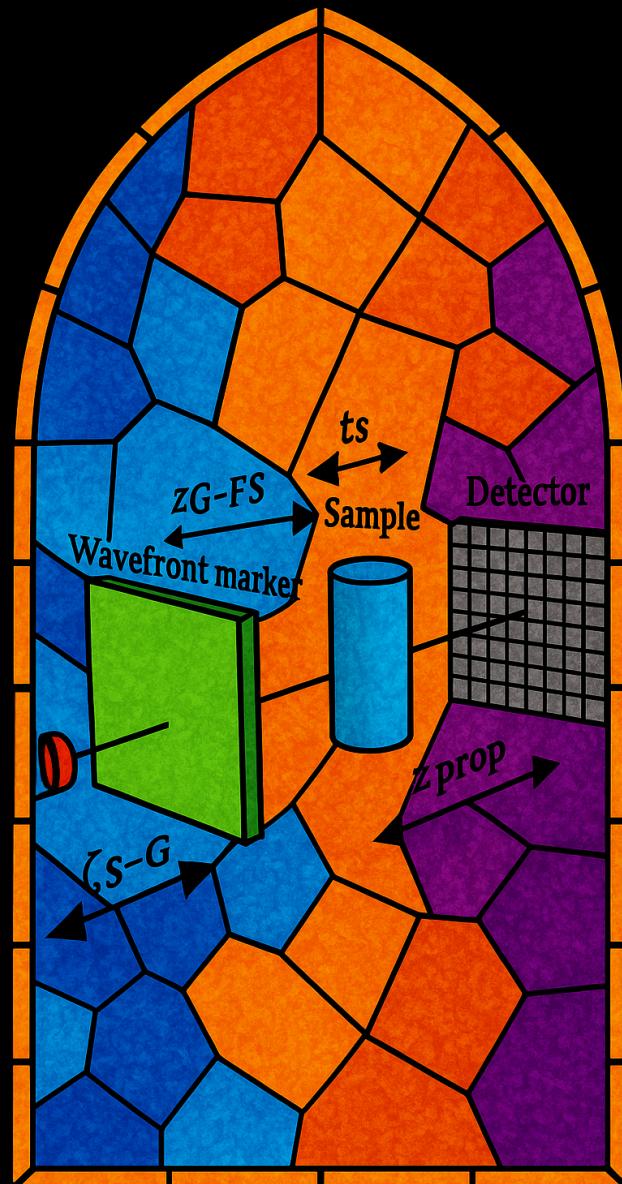


Brief Course on X-Ray Physics



Manuel Fernando Sánchez Alarcón

Chapter 2: Propagation of X-Rays

Derivation of Fresnel propagator

Let's begin with the wave equation (for the electric field associated to an X-ray beam propagating inside a uniform material)

$$\begin{aligned}\nabla^2 \vec{E}(\vec{r}, t) &= \frac{1}{\nu^2} \frac{\partial^2 \vec{E}(\vec{r}, t)}{\partial t^2} \\ &= \frac{n(E)}{c^2} \frac{\partial^2 \vec{E}(\vec{r}, t)}{\partial t^2}\end{aligned}$$

where $\vec{E}(\vec{r}, t)$ is the electric field, ν is the speed of light within a uniform material with refractive index $n(E)$, E is the energy of the X-rays and \vec{r} is the position vector.

Assuming monochromatic plane waves: $\vec{E}(\vec{r}, t) = \psi(\vec{r}) e^{-i\omega t} \hat{e}$, where $\psi(\vec{r})$ is a scalar function, $\omega = \frac{E}{\hbar}$ and \hat{e} is the unit vector that indicates the direction of oscillation of the electric field.

Then:

$$\begin{aligned}\nabla^2 \vec{E}(\vec{r}, t) &= (\nabla^2 \psi(\vec{r})) e^{-i\omega t} \hat{e} \\ \frac{\partial^2 \vec{E}(\vec{r}, t)}{\partial t^2} &= -\psi(\vec{r}) \omega^2 e^{-i\omega t} \hat{e}\end{aligned}$$

$$\Rightarrow (\nabla^2 \psi(\vec{r})) e^{-i\omega t} \vec{e} = -\frac{n^2(\epsilon)}{c^2} \omega^2 \psi(\vec{r}) e^{-i\omega t} \vec{e}$$

$$\Rightarrow \nabla^2 \psi(\vec{r}) + \frac{n^2(\epsilon) \omega^2}{c^2} \psi(\vec{r}) = 0$$

$$\Rightarrow \nabla^2 \psi(\vec{r}) + n^2(\epsilon) k^2 \psi(\vec{r}) = 0$$

(Helmholtz Equation)

where $k = \frac{\omega}{c} = \frac{2\pi}{\lambda}$.

Since electric field was assumed a plane wave and if we assume the photon beam propagates along the z-axis:

$$\psi(\vec{r}) = \psi_0(\vec{r}) e^{in(\epsilon)kz}$$

where $\psi_0(\vec{r})$ is a scalar function. Then:

$$\Rightarrow \nabla^2 (\psi_0(\vec{r}) e^{in(\epsilon)kz}) + n^2(\epsilon) k^2 \psi_0(\vec{r}) e^{in(\epsilon)kz} = 0$$

$$\Rightarrow e^{in(\epsilon)kz} \frac{\partial^2 \psi_0}{\partial x^2} + e^{in(\epsilon)kz} \frac{\partial^2 \psi_0}{\partial y^2} + \frac{\partial^2}{\partial z^2} (\psi_0(\vec{r}) e^{in(\epsilon)kz}) + n^2(\epsilon) k^2 \psi_0(\vec{r}) e^{in(\epsilon)kz} = 0$$

$$\Rightarrow e^{in(\epsilon)kz} \left(\underbrace{\frac{\partial^2 \psi_0}{\partial x^2} + \frac{\partial^2 \psi_0}{\partial y^2}}_{\nabla_\perp^2 \psi_0(\vec{r})} + \frac{\partial}{\partial z} \left(\frac{\partial \psi_0}{\partial z} e^{in(\epsilon)kz} + \psi_0 \cdot i n(\epsilon) k e^{in(\epsilon)kz} \right) + n^2(\epsilon) k^2 \psi_0(\vec{r}) e^{in(\epsilon)kz} \right) = 0$$

$$\Rightarrow e^{in(E)Kz} \nabla_{\perp}^2 \psi_o(\vec{r}) + \frac{\partial^2 \psi_o}{\partial z^2} e^{in(E)Kz} + \frac{\partial \psi_o}{\partial z} in(E)Ke^{in(E)Kz} + \frac{\partial \psi_o}{\partial z} in(E)Ke^{in(E)Kz}$$

$$- \psi_o n^2(E) K^2 e^{in(E)Kz} + n^2(E) K^2 \psi_o e^{in(E)Kz} = 0$$

$$\Rightarrow e^{in(E)Kz} \nabla_{\perp}^2 \psi_o(\vec{r}) + \frac{\partial^2 \psi_o}{\partial z^2} e^{in(E)Kz} + 2 \frac{\partial \psi_o}{\partial z} in(E)Ke^{in(E)Kz} = 0$$

$$\Rightarrow \nabla_{\perp}^2 \psi_o(\vec{r}) + \frac{\partial^2 \psi_o}{\partial z^2} + 2 \frac{\partial \psi_o}{\partial z} in(E)K = 0$$

In the near-field regime, the paraxial approximation is applied:

$$\left| \frac{\partial^2 \psi_o}{\partial z^2} \right| \ll \left| 2 in(E)K \frac{\partial \psi_o}{\partial z} \right| \quad (\text{Slowly-varying } \psi_o)$$

$$\Rightarrow \nabla_{\perp}^2 \psi_o(\vec{r}) + 2 \frac{\partial \psi_o}{\partial z} in(E)K = 0 \quad (\text{Helmholtz paraxial Equation})$$

Let's find a solution. Apply Fourier transform over the transverse plane (x, y):

$$- (k_x^2 + k_y^2) \tilde{F}_{\psi_o} \{ \psi_o(\vec{r}) \} + 2 in(E)K \frac{\partial}{\partial z} \tilde{F}_{\psi_o} \{ \psi_o(\vec{r}) \} = 0$$

$$\underbrace{\tilde{\psi}_o(k_x, k_y, z)}_{= \tilde{\psi}_o} = \tilde{\psi}_o$$

$$\Rightarrow \frac{\partial}{\partial z} \tilde{\psi}_o = \frac{(k_x^2 + k_y^2)}{2im(E)k} \tilde{\psi}_o$$

$$\Rightarrow \tilde{\psi}_o(k_x, k_y, z) = \tilde{\psi}_o(k_x, k_y, z=0) e^{\frac{(k_x^2 + k_y^2)z}{2im(E)k}}$$

Since $\mathcal{F}_{2D}\{\tilde{\psi}_o(\vec{r})\} = \tilde{\psi}_o(k_x, k_y, z) \Rightarrow \mathcal{F}_{2D}^{-1}\{\tilde{\psi}_o(k_x, k_y, z)\} = \psi_o(\vec{r})$

$$\Rightarrow \mathcal{F}_{2D}^{-1}\{\tilde{\psi}_o(k_x, k_y, z)\} = \mathcal{F}_{2D}^{-1}\{\tilde{\psi}_o(k_x, k_y, z=0)\} e^{\frac{(k_x^2 + k_y^2)z}{2im(E)k}}$$

$$\Rightarrow \psi_o(\vec{r}) = \mathcal{F}_{2D}^{-1}\{\tilde{\psi}_o(k_x, k_y, z=0)\} e^{\frac{(k_x^2 + k_y^2)z}{2im(E)k}}$$

Given that $\mathcal{F}\{f \cdot g\} = \mathcal{F}\{f\} \otimes \mathcal{F}\{g\}$

Convolution

$$\Rightarrow \psi_o(\vec{r}) = \mathcal{F}_{2D}^{-1}\{\tilde{\psi}_o(k_x, k_y, z=0)\} \otimes \mathcal{F}_{2D}^{-1}\{e^{\frac{(k_x^2 + k_y^2)z}{2im(E)k}}\}$$

$$= \psi_o(x, y, z=0) \otimes \mathcal{F}_{2D}^{-1}\{e^{\frac{(k_x^2 + k_y^2)z}{2im(E)k}}\}$$

$$= \psi_o(x, y, z=0) \otimes \mathcal{F}_{2D}^{-1}\left\{e^{\frac{k_x^2 z}{2im(E)k}} e^{\frac{k_y^2 z}{2im(E)k}}\right\}$$

Depends only
on k_x only
on k_y

$$= \psi_o(x, y, z=0) \otimes \mathcal{F}_{1D}^{-1}\left\{e^{\frac{k_x^2 z}{2im(E)k}}\right\} \mathcal{F}_{1D}^{-1}\left\{e^{\frac{k_y^2 z}{2im(E)k}}\right\}$$

$$= \psi_o(x, y, z=0) \otimes \mathcal{F}_{1D}^{-1}\left\{e^{\frac{-ik_x^2 z}{2im(E)k}}\right\} \mathcal{F}_{1D}^{-1}\left\{e^{\frac{-ik_y^2 z}{2im(E)k}}\right\}$$

Since

$$\mathcal{F}_{10} \left\{ e^{-ax^2} \right\} = \sqrt{\frac{\pi}{a}} e^{-\frac{k_x^2}{4a}}$$

$$\Rightarrow \mathcal{F}_{10}^{-1} \left\{ e^{-\frac{k_x^2}{4a}} \right\} = \sqrt{\frac{a}{\pi}} e^{-ax^2}$$

$$\text{Identify: } \frac{1}{4a} = \frac{i\tau}{2n(\epsilon)K} \Rightarrow a = \frac{n(\epsilon)K}{2i\tau}$$

$$\begin{aligned} \Rightarrow \psi_o(\vec{r}) &= \psi_o(x, y, z=0) \otimes \left[\left(\sqrt{\frac{n(\epsilon)K}{2\pi i\tau}} \right) e^{-\frac{n(\epsilon)K}{2i\tau}x^2} \left(\sqrt{\frac{n(\epsilon)K}{2\pi i\tau}} \right) e^{-\frac{n(\epsilon)K}{2i\tau}y^2} \right] \\ &= \psi_o(x, y, z=0) \otimes \left[\frac{n(\epsilon)K}{2\pi i\tau} e^{-\frac{n(\epsilon)K}{2i\tau}(x^2 + y^2)} \right] \\ &= \psi_o(x, y, z=0) \otimes \left[\frac{n(\epsilon)K}{2\pi i\tau} \frac{2\pi}{\lambda} e^{\frac{i n(\epsilon)K}{2\tau}(x^2 + y^2)} \right] \\ &= \psi_o(x, y, z=0) \otimes \left[\frac{n(\epsilon)}{i\tau} e^{\frac{i n(\epsilon)K}{2\tau}(x^2 + y^2)} \right] \end{aligned}$$

H(x, y, z) : Fresnel propagator

$$\Rightarrow \psi_o(\vec{r}) = \frac{n(\epsilon)}{i\tau} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi_o(x', y', z=0) e^{\frac{i n(\epsilon)K}{2\tau} [(x-x')^2 + (y-y')^2]} dx' dy'$$

Since $\Psi(\vec{r}) = \Psi_0(\vec{r}) e^{i n(E) k z}$ and hence $\Psi(x, y, z=0) = \Psi_0(x, y, z=0)$

$$\Rightarrow \Psi(\vec{r}) = [\Psi(x, y, z=0) \otimes \left[\frac{n(E)}{i \lambda z} e^{\frac{i n(E) k}{\lambda z} (x^2 + y^2)} \right]] e^{i n(E) k z}$$

$$\Rightarrow \Psi(\vec{r}) = \frac{n(E) e^{i n(E) k z}}{i \lambda z} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Psi(x', y', z=0) e^{\frac{i n(E) k}{\lambda z} [(x-x')^2 + (y-y')^2]} dx' dy'$$

(Fresnel Diffraction Integral)

In simple words: If you have an initial wavefield $\Psi(x, y, z=0)$ and you want to propagate it across a material with refractive index $n(E)$ to a position z along the propagation axis, then the propagated wavefield $\Psi(\vec{r})$ is $\Psi(\vec{r}) = \Psi(x, y, z=0) \otimes H(x, y, z)$

• In vacuum: $n(E) = 1$. In air $n(E) \approx 1$.

Transport of Intensity Equation (TIE):

Let's begin with the Helmholtz paraxial equation:

$$\nabla_{\perp}^2 \Psi_0(\vec{r}) + 2 \frac{\partial \Psi_0}{\partial z} i n(E) k = 0$$

To make things easy, let's consider $n(E) = 1$ (vacuum or air).

Since $\psi_0(\vec{r})$ is a complex number, then we can write it as

$$\psi_0(\vec{r}) = A(\vec{r}) e^{i\phi(\vec{r})}$$

$$\Rightarrow \nabla^2 \left(A(\vec{r}) e^{i\phi(\vec{r})} \right) + 2 \frac{\partial}{\partial z} \left(A(\vec{r}) e^{i\phi(\vec{r})} \right) ik = 0$$

$$\Rightarrow \frac{\partial^2}{\partial x^2} (A e^{i\phi}) + \frac{\partial^2}{\partial y^2} (A e^{i\phi}) + 2 \frac{\partial}{\partial z} (A e^{i\phi}) ik = 0$$

$$\Rightarrow \frac{\partial}{\partial x} \left(\frac{\partial A}{\partial x} e^{i\phi} + A i \frac{\partial \phi}{\partial x} e^{i\phi} \right) + \frac{\partial}{\partial y} \left(\frac{\partial A}{\partial y} e^{i\phi} + A i \frac{\partial \phi}{\partial y} e^{i\phi} \right) + 2 \frac{\partial A}{\partial z} e^{i\phi} ik - 2 A k \frac{\partial \phi}{\partial z} e^{i\phi} = 0$$

$$\Rightarrow \cancel{\frac{\partial^2 A}{\partial x^2} e^{i\phi}} + \cancel{\frac{\partial A}{\partial x} i \frac{\partial \phi}{\partial x} e^{i\phi}} + i \cancel{\frac{\partial A}{\partial x} \frac{\partial \phi}{\partial x} e^{i\phi}} + i A \cancel{\frac{\partial^2 \phi}{\partial x^2} e^{i\phi}} - A \cancel{\left(\frac{\partial \phi}{\partial x} \right)^2 e^{i\phi}} + \dots$$

$$\dots \cancel{\frac{\partial^2 A}{\partial y^2} e^{i\phi}} + \cancel{\frac{\partial A}{\partial y} i \frac{\partial \phi}{\partial y} e^{i\phi}} + i \cancel{\frac{\partial A}{\partial y} \frac{\partial \phi}{\partial y} e^{i\phi}} + i A \cancel{\frac{\partial^2 \phi}{\partial y^2} e^{i\phi}} - A \cancel{\left(\frac{\partial \phi}{\partial y} \right)^2 e^{i\phi}} + \dots$$

$$\dots 2 \cancel{\frac{\partial A}{\partial z} e^{i\phi}} ik - 2 A k \cancel{\frac{\partial \phi}{\partial z} e^{i\phi}} = 0$$

$$\Rightarrow \frac{\partial^2 A}{\partial x^2} + 2i \frac{\partial A}{\partial x} \frac{\partial \phi}{\partial y} + i A \frac{\partial^2 \phi}{\partial x^2} - A \left(\frac{\partial \phi}{\partial x} \right)^2 + \frac{\partial^2 A}{\partial y^2} + 2i \frac{\partial A}{\partial y} \frac{\partial \phi}{\partial x} + i A \frac{\partial^2 \phi}{\partial y^2} - A \left(\frac{\partial \phi}{\partial y} \right)^2$$

$$+ 2ik \frac{\partial A}{\partial z} - 2Ak \frac{\partial \phi}{\partial z} = 0$$

Since

$$I(\vec{r}) = |\Psi_0(\vec{r})|^2 = A(\vec{r}) \rightarrow A(\vec{r}) = \sqrt{I(\vec{r})}$$

$$\rightarrow \frac{\partial I}{\partial x} = 2A \frac{\partial A}{\partial x}, \quad \frac{\partial I}{\partial y} = 2A \frac{\partial A}{\partial y}, \quad \frac{\partial I}{\partial z} = 2A \frac{\partial A}{\partial z}$$

$$\rightarrow \frac{\partial^2 I}{\partial x^2} = 2\left(\frac{\partial A}{\partial x}\right)^2 + 2A \frac{\partial^2 A}{\partial x^2}, \quad \frac{\partial^2 I}{\partial y^2} = 2\left(\frac{\partial A}{\partial y}\right)^2 + 2A \frac{\partial^2 A}{\partial y^2}$$

Assuming slowly-varying Intensity:

$$\frac{\partial^2 A}{\partial x^2} \approx \frac{\partial^2 A}{\partial y^2} \approx \left(\frac{\partial A}{\partial x}\right)^2 \approx \left(\frac{\partial A}{\partial y}\right)^2 \approx 0$$

$$\Rightarrow \frac{\partial^2 I}{\partial x^2} \approx 0, \quad \frac{\partial^2 I}{\partial y^2} \approx 0$$

Then:

$$\cancel{\frac{\partial^2 A}{\partial x^2}} + 2i \frac{\partial A}{\partial x} \frac{\partial \phi}{\partial x} + iA \frac{\partial^2 \phi}{\partial x^2} - A \left(\frac{\partial \phi}{\partial x}\right)^2 + \cancel{\frac{\partial^2 A}{\partial y^2}} + 2i \frac{\partial A}{\partial y} \frac{\partial \phi}{\partial y} + iA \frac{\partial^2 \phi}{\partial y^2} - A \left(\frac{\partial \phi}{\partial y}\right)^2$$

$$+ 2ik \frac{\partial A}{\partial z} - 2Ak \frac{\partial \phi}{\partial z} = 0$$

$$\Rightarrow 2i \frac{1}{2\sqrt{I}} \frac{\partial I}{\partial x} \frac{\partial \phi}{\partial x} + i\sqrt{I} \frac{\partial^2 \phi}{\partial x^2} - \sqrt{I} \left(\frac{\partial \phi}{\partial x}\right)^2 + 2i \frac{1}{2\sqrt{I}} \frac{\partial I}{\partial y} \frac{\partial \phi}{\partial y} + i\sqrt{I} \frac{\partial^2 \phi}{\partial y^2} - \sqrt{I} \left(\frac{\partial \phi}{\partial y}\right)^2$$

$$+ 2ik \frac{1}{2\sqrt{I}} \frac{\partial I}{\partial z} - 2\sqrt{I} k \frac{\partial \phi}{\partial z} = 0$$

Multiplying by \sqrt{I} :

$$\Rightarrow i \frac{\partial I}{\partial x} \frac{\partial \phi}{\partial x} + i I \frac{\partial^2 \phi}{\partial x^2} - I \left(\frac{\partial \phi}{\partial x} \right)^2 + i \frac{\partial I}{\partial y} \frac{\partial \phi}{\partial y} + i I \frac{\partial^2 \phi}{\partial y^2} - I \left(\frac{\partial \phi}{\partial y} \right)^2 + i \kappa \frac{\partial I}{\partial z} - 2 I \kappa \frac{\partial \phi}{\partial z} = 0$$

Dividing by i :

$$\Rightarrow \frac{\partial I}{\partial x} \frac{\partial \phi}{\partial x} + I \frac{\partial^2 \phi}{\partial x^2} - \frac{1}{i} I \left(\frac{\partial \phi}{\partial x} \right)^2 + \frac{\partial I}{\partial y} \frac{\partial \phi}{\partial y} + I \frac{\partial^2 \phi}{\partial y^2} - \frac{1}{i} I \left(\frac{\partial \phi}{\partial y} \right)^2 + \kappa \frac{\partial I}{\partial z} - \frac{2}{i} I \kappa \frac{\partial \phi}{\partial z} = 0$$

$$\Rightarrow \frac{\partial I}{\partial x} \frac{\partial \phi}{\partial x} + I \frac{\partial^2 \phi}{\partial x^2} + i I \left(\frac{\partial \phi}{\partial x} \right)^2 + \frac{\partial I}{\partial y} \frac{\partial \phi}{\partial y} + I \frac{\partial^2 \phi}{\partial y^2} + i I \left(\frac{\partial \phi}{\partial y} \right)^2 + \kappa \frac{\partial I}{\partial z} + 2i I \kappa \frac{\partial \phi}{\partial z} = 0$$

$$\Rightarrow -\kappa \frac{\partial I}{\partial z} = \left[\frac{\partial I}{\partial x} \frac{\partial \phi}{\partial x} + \frac{\partial I}{\partial y} \frac{\partial \phi}{\partial y} + I \frac{\partial^2 \phi}{\partial x^2} + I \frac{\partial^2 \phi}{\partial y^2} \right] + i \left[I \left(\frac{\partial \phi}{\partial x} \right)^2 + I \left(\frac{\partial \phi}{\partial y} \right)^2 + 2i I \kappa \frac{\partial \phi}{\partial z} \right]$$

$$\Rightarrow -\kappa \frac{\partial I}{\partial z} = \left[\left(\frac{\partial I}{\partial x}, \frac{\partial I}{\partial y} \right) \cdot \left(\frac{\partial \phi}{\partial x}, \frac{\partial \phi}{\partial y} \right) + I \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right) \right] + i I \left[\left(\frac{\partial \phi}{\partial x} \right)^2 + \left(\frac{\partial \phi}{\partial y} \right)^2 + 2i \kappa \frac{\partial \phi}{\partial z} \right]$$

$$\Rightarrow -\kappa \frac{\partial I}{\partial z} = \left[\nabla_I \cdot \nabla_{\perp} \phi + I \nabla_{\perp}^2 \phi \right] + i I \left[\left(\frac{\partial \phi}{\partial x} \right)^2 + \left(\frac{\partial \phi}{\partial y} \right)^2 + 2i \kappa \frac{\partial \phi}{\partial z} \right]$$

Since $K, I \in \mathbb{R}$, then $I_m(-K \frac{\partial I}{\partial z}) = 0$, Then

$$\left(\frac{\partial \phi}{\partial x}\right)^2 + \left(\frac{\partial \phi}{\partial y}\right)^2 + 2K \frac{\partial \phi}{\partial z} = 0$$

and:

$$-K \frac{\partial I}{\partial z} = I(\vec{r}) \nabla_{\perp}^2 \phi(\vec{r}) + \nabla_{\perp} I(\vec{r}) \cdot \nabla_{\perp} \phi(\vec{r}) \quad (\text{TE})$$

For a pure-phase object it is assured $I(\vec{r}) = I_o(z)$ (constant with respect to (x, y))

Then:

$$-K \frac{dI_o(z)}{dt} = I_o(z) \nabla_{\perp}^2 \phi(\vec{r})$$

Assuming $\phi(\vec{r}) = \phi(x, y)$ (Phase map):

$$\Rightarrow \int_{I_o(t=0)}^{I_o(t)} \frac{dI_o'(t)}{I_o'(t)} dt = - \frac{\nabla_{\perp}^2 \phi(x, y)}{K} \int_{z=0}^z dz'$$

$$\Rightarrow \ln \left(\frac{I_o(t)}{I_o(t=0)} \right) = - \frac{\nabla_{\perp}^2 \phi(x, y)}{K} z$$

$$\Rightarrow I_o(t) = I_o(t=0) e^{-\frac{\nabla_{\perp}^2 \phi(x,y)}{k} z}$$

For X-rays: $\frac{\nabla_{\perp}^2 \phi(x,y)}{k} \ll 1$

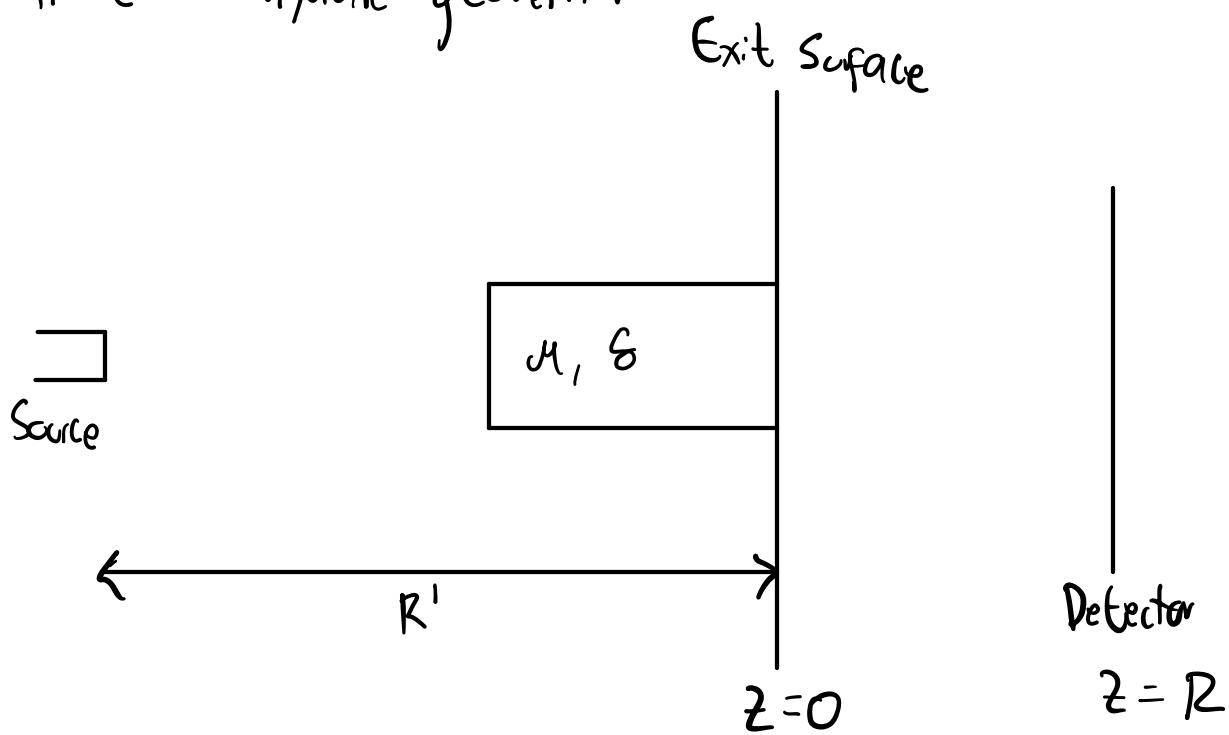
$$\Rightarrow I_o(t) \approx I_o(t=0) \left[1 - \frac{z}{k} \nabla_{\perp}^2 \phi(x,y) \right]$$

Chapter 3: Phase Retrieval (Paganin)

De la última clase:

$$\begin{aligned} -\kappa \frac{\partial I(\vec{r})}{\partial z} &= I(\vec{r}) \nabla_{\perp}^2 \phi(x,y) + \nabla_{\perp} I(\vec{r}) \cdot \nabla_{\perp} \phi(x,y) \\ &= \nabla_{\perp} \cdot (I(\vec{r}) \nabla_{\perp} \phi(x,y)) \end{aligned}$$

Considera la siguiente geometría:



Dado q-e:

- $I(x,y, z=0) = \int_{\text{no samp}} e^{-\mu t(x,y)}$ No integral Projection - Approximation
(Beer - Lambert)
- $\phi(x,y) = -S \kappa t(x,y)$
- $\frac{\partial I(x,y, z=0)}{\partial z} \approx \frac{I(x,y, z=R) - I(x,y, z=0)}{R} = \frac{I(x,y, z=R) - I_{\text{no samp}} e^{-\mu t(x,y)}}{R}$

$$\Rightarrow \frac{(\nabla I(E)) - k^2}{\partial z} I(x,y, z=0) = \nabla_{\perp} (I(x,y, z=0) \nabla_{\perp} \phi(x,y))$$

$$\Rightarrow \frac{\cancel{\nabla}_{\perp} (I(x,y, z=R) - I_{no\ samp} e^{-\mu t(x,y)})}{R} = \nabla_{\perp} (I_{no\ samp} e^{-\mu t(x,y)} \nabla_{\perp} (\cancel{\phi(x,y)}))$$

$$\begin{aligned} \Rightarrow I(x,y, z=R) - I_{no\ samp} e^{-\mu t(x,y)} &= \frac{\delta R}{\mu} I_{no\ samp} \nabla_{\perp} \cdot (e^{-\mu t(x,y)} \nabla_{\perp} t(x,y)) \\ &= \frac{\delta R}{\mu} I_{no\ samp} \nabla_{\perp} \cdot \left(e^{-\mu t(x,y)} - \frac{1}{\mu} \nabla_{\perp} (-\mu t(x,y)) \right) \\ &= -\frac{\delta R}{\mu} I_{no\ samp} \nabla_{\perp} \cdot (e^{-\mu t(x,y)} \nabla_{\perp} (-\mu t(x,y))) \\ &= -\frac{\delta R}{\mu} I_{no\ samp} \nabla_{\perp} \cdot (\nabla_{\perp} e^{-\mu t(x,y)}) \\ &= -\frac{\delta R}{\mu} I_{no\ samp} \nabla_{\perp}^2 e^{-\mu t(x,y)} \end{aligned}$$

$$\Rightarrow I(x,y, z=R) = I_{no\ samp} \left(e^{-\mu t(x,y)} - \frac{\delta R}{\mu} \nabla_{\perp}^2 e^{-\mu t(x,y)} \right)$$

$$\Rightarrow \frac{I(x,y, z=0)}{I_{no\ samp}} = e^{-\mu t(x,y)} - \frac{\delta R}{\mu} \nabla_{\perp}^2 e^{-\mu t(x,y)}$$

Necesitamos despejar $t(x,y)$!

⇒ Usar transformador de Fourier 2D sobre (x, y) :

$$\mathcal{F}_{2D} \left\{ \frac{I(x, y, z=0)}{I_{no\ scan}} \right\} = \mathcal{F}_{2D} \left\{ e^{-ut(x, y)} \right\} - \frac{\delta R}{\mu} (-k_x^2 - k_y^2) \mathcal{F}_{2D} \left\{ e^{-ut(x, y)} \right\}$$

$$= \left[1 + \frac{\delta R}{\mu} (k_x^2 + k_y^2) \right] \mathcal{F}_{2D} \left\{ e^{-ut(x, y)} \right\}$$

$$\Rightarrow \mathcal{F}_{2D} \left\{ e^{-ut(x, y)} \right\} = \frac{1}{1 + \frac{\delta R}{\mu} \underbrace{(k_x^2 + k_y^2)}_{= k_\perp^2}} \mathcal{F}_{2D} \left\{ \frac{I(x, y, z=0)}{I_{no\ scan}} \right\}$$

$$= \frac{1}{1 + \frac{\delta R}{\mu} k_\perp^2} \mathcal{F}_{2D} \left\{ \frac{I(x, y, z=0)}{I_{no\ scan}} \right\}$$

$$\Rightarrow e^{-ut(x, y)} = \mathcal{F}_{2D}^{-1} \left\{ \frac{1}{1 + \frac{\delta R}{\mu} k_\perp^2} \mathcal{F}_{2D} \left\{ \frac{I(x, y, z=0)}{I_{no\ scan}} \right\} \right\}$$

$$\Rightarrow t(x, y) = -\frac{1}{\mu} \ln \left[\mathcal{F}_{2D}^{-1} \left\{ \frac{1}{1 + \frac{\delta R}{\mu} k_\perp^2} \mathcal{F}_{2D} \left\{ \frac{I(x, y, z=0)}{I_{no\ scan}} \right\} \right\} \right]$$

$$\Rightarrow \phi(x, y) = \frac{\delta R}{\mu} \ln \left[\mathcal{F}_{2D}^{-1} \left\{ \frac{1}{1 + \frac{\delta R}{\mu} k_\perp^2} \mathcal{F}_{2D} \left\{ \frac{I(x, y, z=0)}{I_{no\ scan}} \right\} \right\} \right]$$

Esta expresión es válida para rayos paralelos ($R' \rightarrow \infty$).

Si consideramos que beam (efectos de magnificación), el fresnel scaling theorem indica:

$$I_{\text{mag}}(x, y, z) = \frac{1}{M^2} I\left(\frac{x}{M}, \frac{y}{M}, \frac{z}{M}\right)$$

Con $M = \frac{R' + R}{R'}$ la magnificación. Luego:

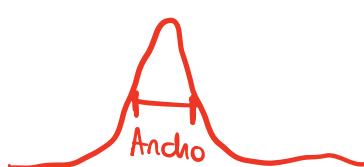
$$\Rightarrow t(x, y) = -\frac{1}{\mu} \ln \left[F_{20}^{-1} \left\{ \frac{1}{1 + \frac{\sigma}{\mu} \frac{R}{M} k_{\perp}^2} F_{20} \right\} \frac{M^2 I_{\text{mag}}(Mx, My, z=R)}{I_{\text{av samp, mag}}} \right]$$

Meaning:

$$t(x, y) = -\frac{1}{\mu} \ln \left[F_{20}^{-1} \left\{ \underbrace{\frac{1}{1 + \frac{\sigma}{\mu} \frac{R}{M} k_{\perp}^2}}_{\text{Low-pass filter on Fourier domain}} F_{20} \right\} \underbrace{\frac{M^2 I_{\text{mag}}(Mx, My, z=R)}{I_{\text{av samp, mag}}}}_{\text{Flat-field corrected image}} \right]$$

Low-pass filter
on Fourier domain

Flat-field corrected
image



Ancho: Depende de $\frac{\sigma}{\mu} \frac{R}{M}$

¿Por qué necesitamos distancias con defectos grandes para notar efectos de fase?

Ley de Snell:

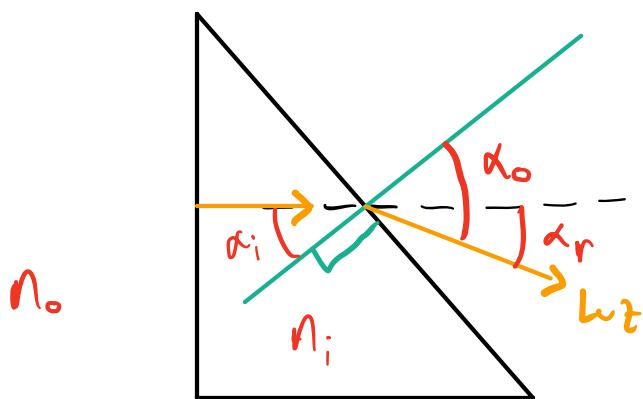
$$n_i \sin \underline{\alpha_i} = n_o \sin \underline{\alpha_o}$$

Ángulo de
incidencia

Ángulo de
Salida

$$(\underline{\alpha_r} = \underline{\alpha_o} - \underline{\alpha_i})$$

Ángulo de
refracción.



Para ángulos pequeños:

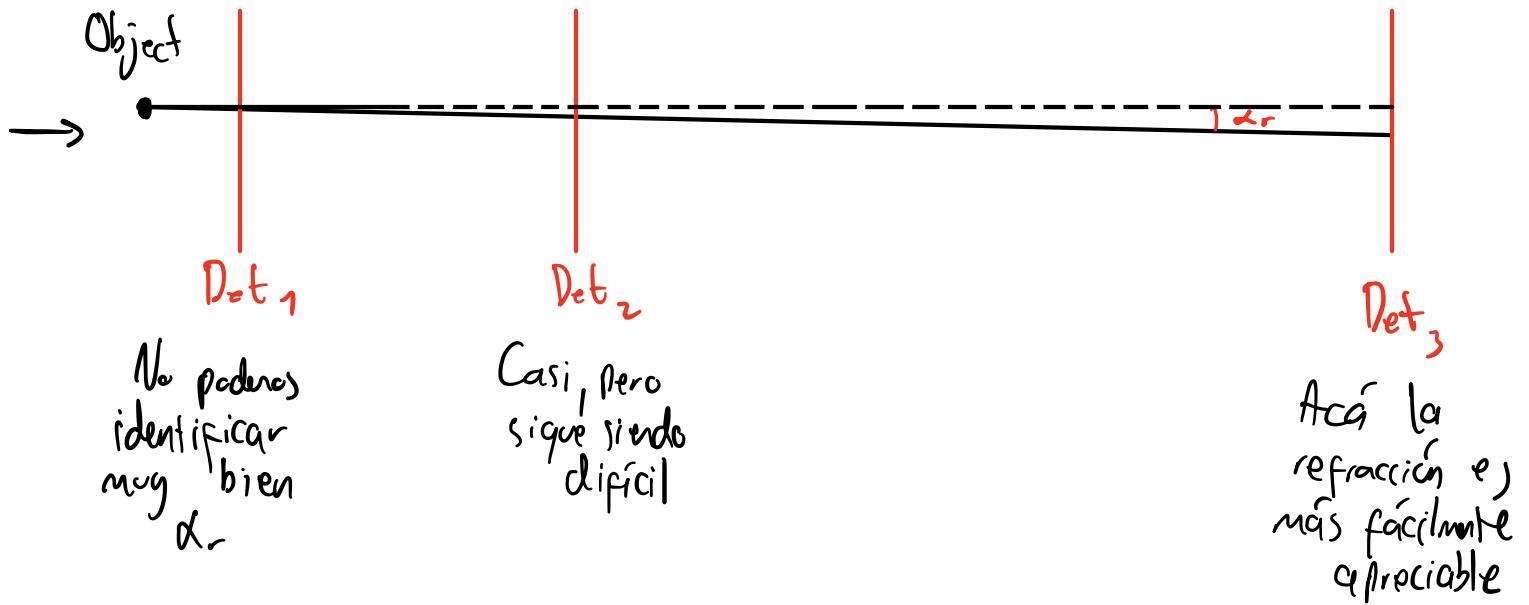
$$n_i \alpha_i \approx n_o \alpha_o$$

Supongamos $n_o = 1$ (Vacio, \sim aire)

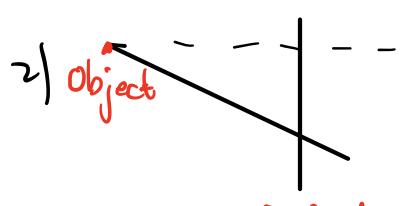
$$n_i \alpha_i \approx \alpha_o$$

$$\rightarrow \alpha_r = \alpha_o - \alpha_i = n_i \alpha_i - \alpha_i = (n_i - 1) \alpha_i$$

Para rayos X $|n_i|$ es muy cercana a 1, luego n_{i-1} es muy cercano a 0 y α_r es MUY pequeño. En luz visible este no es un problema \rightarrow Refracción (efecto de fase) pueden ser visibles fácilmente.



1) $\alpha_r \sim \mu_{\text{rad}}$

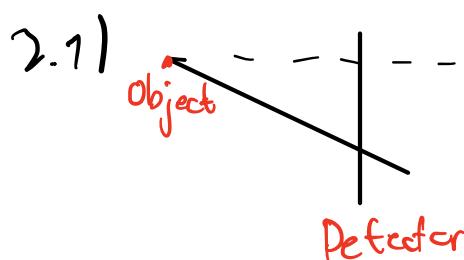


Propagation distance = $\frac{10^{-3} \text{ m}}{\tan \alpha_r} \approx \frac{10^{-3} \text{ m}}{\alpha_r}$

(objeto a detector)

$1 \text{ mm} = 10^{-3} \text{ m} \rightarrow$

$\approx \frac{10^{-3} \text{ m}}{10^{-6} \text{ rad}} \sim 10^3 \text{ m}$



$1 \text{ dm} = 10^{-1} \text{ m} \rightarrow$ Prop. distance $\sim 1 \text{ m}$

¿Cómo medir α_r de forma fácil sin necesidad de tener distancias de propagación tan grandes?

Chapter 4: Fokker-Planck X-ray Equation (Path Integral Formulation)

A Path-Integral Way to Understand X-ray Multimodal X-ray Imaging

Manuel Fernando Sánchez Alarcón^{1,*}

¹Physics Department, Universidad de los Andes, Bogotá, Colombia

*Corresponding author: mf.sanchez17@uniandes.edu.co

Abstract

In this article, the path-integral formalism is introduced to explain the physics behind various X-ray multimodal imaging techniques using grating interferometry.

Keywords: Path integral, X-ray.

Nomenclature

k Wave number

$I(x, z)$ Intensity

$\int \mathcal{D}x$ The functional integral. Also represented by $\int \mathcal{D}[x(z)]$

1. Introduction

2. Path-Integral from X-ray interactions

Consider the scenario shown in Fig. 1, where a non-polarized monochromatic X-ray plane wave interacts with a sample whose refractive index $n_s(x, z) = n_s$ is assumed to be constant. Also, assume that the X-ray wave travels in vacuum (where the refractive index is $n_v(x, y) = 1$, and at a certain point in time, a photon interacts with the sample at the point (x_0, z_0) . Additionally, assume that the X-ray plane wave can be described by a scalar theory, allowing the X-ray photon interactions to be represented by a single scalar wave function $\psi(x, z)$.

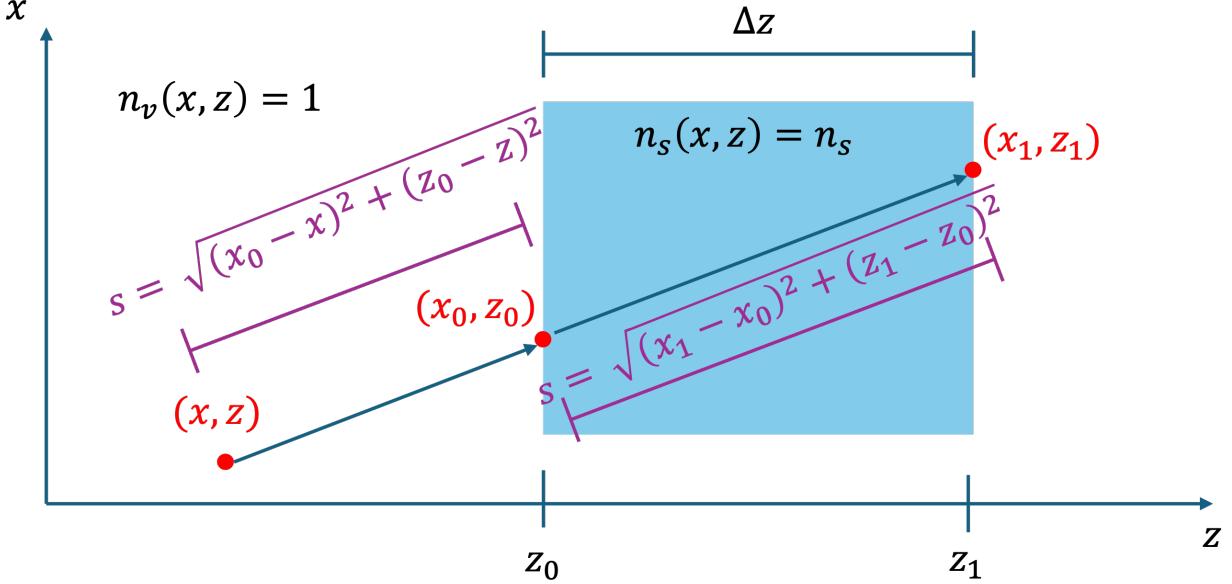


Figure 1: Propagation of a photon inside an homogeneous material of refractive index $n_s(x, y) = n_s$.

For $z \leq z_0^-$, the wave function can be modeled as shown in Eq. (1), where s is the geometrical length of the path that the photon traveled to reach the sample at the point (x_0, z_0) from another point (x, z) in vacuum, k is the wave number, and ψ_0 is a constant which represents the amplitude of the wave.

$$\begin{aligned} \psi(x, z) &= \psi_0 \exp\left(ik \int_{(x,z)}^{(x_0,z_0)} n_v(x, z) ds\right) = \psi_0 \exp\left(ik \int_{(x,z)}^{(x_0,z_0)} ds\right) \\ &= \psi_0 \exp\left(ik \sqrt{(x_0 - x)^2 + (z_0 - z)^2}\right). \end{aligned} \quad (1)$$

Within the material, i.e for $z_0^+ \leq z \leq z_1$, the wave function is described by Eq. 2, where s represents the geometrical length of the path that the photon traveled from the point (x_0, z_0) to any point (x, z) inside the material.

$$\begin{aligned} \psi(x, z) &= \psi_0 \exp\left(ik \int_{(x_0,z_0)}^{(x,z)} n_s(x, z) ds\right) = \psi_0 \exp\left(ik n_s \int_{(x_0,z_0)}^{(x,z)} ds\right) \\ &= \psi_0 \exp\left(ik n_s \sqrt{(x - x_0)^2 + (z - z_0)^2}\right). \end{aligned} \quad (2)$$

Note that $\psi(x_0, z_0^-) = \psi(x_0, z_0^+)$, ensuring continuity between both expressions for the wave function at (x_0, z_0) . Consequently, the constant ψ_0 can be expressed as $\psi_0 = \psi(x_0, z_0)$, and hence, the wave function at (x_1, z_1) can be calculated as:

$$\psi(x_1, z_1) = \exp\left(ik n_s \sqrt{(x_1 - x_0)^2 + \Delta z^2}\right) \psi(x_0, z_0), \quad (3)$$

where $\Delta z = z_1 - z_0$ is the thickness of the material. However, photons interacting at a fixed point (x_0, z_0) are not the only ones that can propagate to the point (x_1, z_1) . To find an expression for $\psi(x_1, z_1)$ that accounts for contributions from photons interacting at N_p different positions $\{x_{0,j}\}_{1 \leq j \leq N_p}$ along the x -axis, we must consider **all possible propagation paths** that end at (x_1, z_1) . Mathematically, this means that a more complete expression for $\psi(x_1, z_1)$ should be:

$$\psi(x_1, z_1) = \sum_{j=1}^{N_p} \exp\left(ikn_s \sqrt{(x_1 - x_{0,j})^2 + \Delta z^2}\right) \psi(x_{0,j}, z_0). \quad (4)$$

By considering not a discrete, but a continuum of possible interaction points, Eq. (4) turns into Eq. (5), where $K_s(x_1, z_1 | x_0, z_0) = \exp\left(ikn_s \sqrt{(x_1 - x_0)^2 + \Delta z^2}\right)$ can be interpreted as an operator which propagates a photon to the point (x_1, z_1) given that such photon interacted with the sample at the point (x_0, z_0) .

$$\psi(x_1, z_1) = \int_{-\infty}^{\infty} dx_0 K_s(x_1, z_1 | x_0, z_0) \psi(x_0, z_0). \quad (5)$$

Now consider the non-uniform sample shown in Fig. 2, described by a non-constant refractive index $n_s(x, z)$. The sample is divided into N parts of thickness $\Delta z = (x_b - x_a)/N$. Additionally, suppose that N is sufficiently large so that each slice can be considered a uniform sample (with a constant refractive index) along the z -axis. Since each slice is now considered a uniform sample, we can apply the result found in Eq. (5) to each slice.

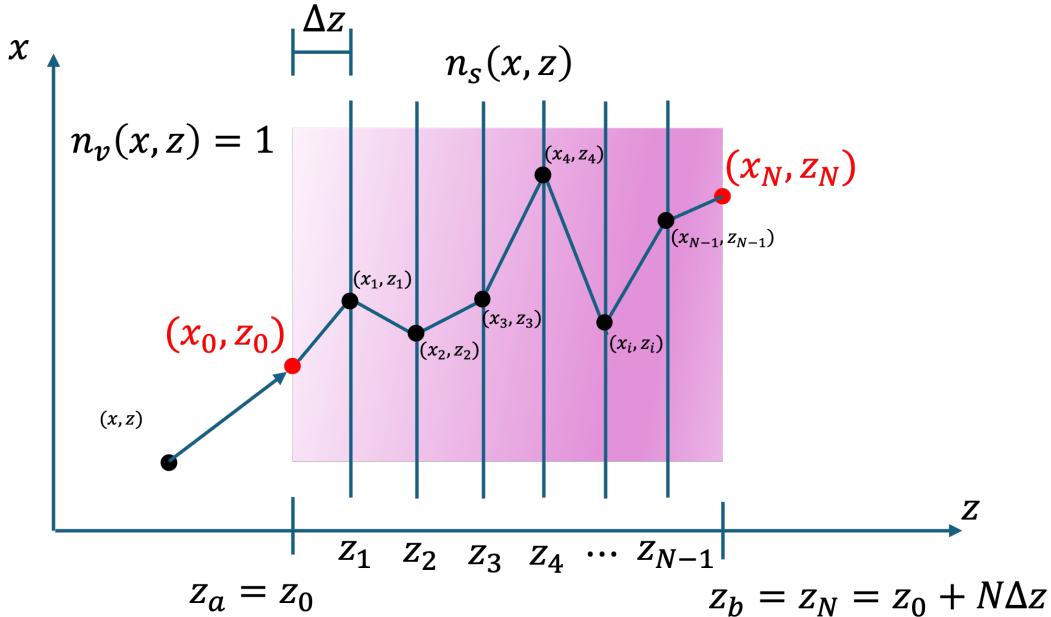


Figure 2: Propagation of a photon inside a non-homogeneous material of refractive index $n_s(x, y)$.

For the first slice, we know that:

$$\psi(x_1, z_1) = \int_{-\infty}^{\infty} dx_0 K_s(x_1, z_1 | x_0, z_0) \psi(x_0, z_0). \quad (6)$$

For the second slice:

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$$\psi(x_2, z_2) = \int_{-\infty}^{\infty} dx_1 K_s(x_2, z_2 | x_1, z_1) \psi(x_1, z_1). \quad (7)$$

In consequence:

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$$\begin{aligned} \psi(x_2, z_2) &= \int_{-\infty}^{\infty} dx_1 K_s(x_2, z_2 | x_1, z_1) \left(\int_{-\infty}^{\infty} dx_0 K_s(x_1, z_1 | x_0, z_0) \psi(x_0, z_0) \right) \\ &= \int_{-\infty}^{\infty} dx_0 \int_{-\infty}^{\infty} dx_1 K_s(x_2, z_2 | x_1, z_1) K_s(x_1, z_1 | x_0, z_0) \psi(x_0, z_0). \end{aligned}$$

By repeating the previous procedure iteratively for each slice, we find that:

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$$\begin{aligned} \psi(x_N, z_N) &= \int_{-\infty}^{\infty} dx_0 \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_{N-1} \prod_{i=1}^N K_s(x_i, z_i | x_{i-1}, z_{i-1}) \psi(x_0, z_0) \\ &= \int_{-\infty}^{\infty} dx_0 K_N(x_N, z_N | x_0, z_0) \psi(x_0, z_0), \end{aligned} \quad (8)$$

where:

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$$\begin{aligned} K_N(x_N, z_N | x_0, z_0) &= \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_{N-1} \prod_{i=1}^N K_s(x_i, z_i | x_{i-1}, z_{i-1}) \\ &= \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_{N-1} \prod_{i=1}^N \exp\left(ikn_s(x_i, z_i)\sqrt{(x_i - x_{i-1})^2 + \Delta z^2}\right) \\ &= \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_{N-1} \exp\left(ik \sum_{i=1}^N n_s(x_i, z_i) \sqrt{(x_i - x_{i-1})^2 + \Delta z^2}\right) \\ &= \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_{N-1} \exp\left(ik \sum_{i=1}^N n_s(x_i, z_i) \sqrt{1 + \left(\frac{x_i - x_{i-1}}{\Delta z}\right)^2} \Delta z\right) \end{aligned}$$

is defined in analogy to $K_s(x_1, z_1 | x_0, z_0)$ in Eq. (5). From a quantum-mechanics point of view, $K_N(x_N, z_N | x_0, z_0)$ represents the probability amplitude associated with a photon propagating to (x_N, z_N) given that it interacted with the sample at (x_0, z_0) . From a practical point of view, this term describes the propagation of a photon from an initial fixed point (x_0, z_0) to a final fixed point (x_N, z_N) . This is why the term is typically referred to as the **propagator**. To ensure the probabilistic nature of $K_N(x_N, z_N | x_0, z_0)$, a normalization constant \mathcal{N} should be added to its definition, so that:

$$K_N(x_N, z_N | x_0, z_0) = \mathcal{N} \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_{N-1} \exp \left(ik \sum_{i=1}^N n_s(x_i, z_i) \sqrt{1 + \left(\frac{x_i - x_{i-1}}{\Delta z} \right)^2} \Delta z \right). \quad (9)$$

In the limit when $N \rightarrow \infty$, we must consider the next correspondences:

$$\begin{aligned} \sum_{i=1}^N n_s(x_i, z_i) \sqrt{1 + \left(\frac{x_i - x_{i-1}}{\Delta z} \right)^2} \Delta z &\rightarrow \int_{z_a}^{z_b} n_s(x, z) \sqrt{1 + \left(\frac{dx}{dz} \right)^2} dz \\ \mathcal{N} \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_{N-1} &\rightarrow \int \mathcal{D}[x(z)] \end{aligned} \quad (10)$$

and, in consequence:

$$\begin{aligned} K(x_b, z_b | x_a, z_a) &= \lim_{N \rightarrow \infty} K_N(x_N, z_N | x_0, z_0) \\ &= \int \mathcal{D}[x(z)] \exp \left(ik \int_{z_a}^{z_b} n_s(x, z) \sqrt{1 + \left(\frac{dx}{dz} \right)^2} dz \right). \end{aligned} \quad (11)$$

The integral form of $K(x_b, z_b | x_a, z_a)$ in Eq. (11) is called a **path integral** or a **functional integral**. The general form of a path integral in physics is shown in Eq. (12), where the functional $S[x, \frac{dx}{dz}]$ is called the action. For the specific example in Fig. 2, the action is $S[x, \frac{dx}{dz}] = k \int_{z_a}^{z_b} n_s(x, z) \sqrt{1 + \left(\frac{dx}{dz} \right)^2} dz$.

$$K(x, z | x', z') = \int \mathcal{D}[x(z)] \exp \left(iS \left[x, \frac{dx}{dz} \right] \right). \quad (12)$$

Typically, the action is expressed in terms of another function called Lagrangian $L(x, \frac{dx}{dz})$, so that:

$$S \left[x, \frac{dx}{dz} \right] = \int_{z'}^z L \left(x, \frac{dx}{dz} \right) dz. \quad (13)$$

For the specific example illustrated in Fig. 2, the Lagrangian is:

$$L \left(x, \frac{dx}{dz} \right) = kn_s(x, z) \sqrt{1 + \left(\frac{dx}{dz} \right)^2}. \quad (14)$$

Considering that $N \rightarrow \infty$, Eq. (8) turns into Eq. (15).

$$\psi(x, z) = \int_{-\infty}^{\infty} dx' K(x, z|x', z') \psi(x', z'). \quad (15)$$

As a side note, Eqs. (12) and (15) are equivalent to the Chapman-Kolmogorov equation 67 and the Evolution equation respectively, which describes a Markov process. Similar expressions can be obtained if no wave functions but intensities are considered. In Appendix 68 69 C it was found that the equivalents to Eqs. (12) and (15) in terms of intensities are: 70

$$I(x, z) = \int_{-\infty}^{\infty} dx' K_I(x, z|x', z') I(x', z'), \quad (16)$$

and: 71

$$K_I(x, z|x', z') = \int_{x(z')=x'}^{x(z)=x} \mathcal{D}x \exp\left(-2 \operatorname{Im}\left(S\left[x, \frac{dx}{dz}\right]\right)\right), \quad (17)$$

respectively. For the example illustrated in Fig. 2, the propagator $K_I(x, z|x', z')$ is given 72 by: 73

$$K_I(x, z|x', z') = \int_{x(z')=x'}^{x(z)=x} \mathcal{D}x \exp\left(-\int_{z'}^z 2k \operatorname{Im}(n_s(x, \tilde{z})) \sqrt{1 + \left(\frac{dx}{d\tilde{z}}\right)^2} d\tilde{z}\right). \quad (18)$$

The complex refractive index $n_s(x, z)$ is typically expressed as $n_s(x, z) = 1 - \delta(x, z) + 74 i\beta(x, z)$, where $\delta(x, z)$ and $\beta(x, z)$ represent the dispersive and absorptive effects in X-ray 75 interactions with matter. Since $\operatorname{Im}(n_s(x, z)) = \beta(x, z)$, then: 76

$$K_I(x, z|x', z') = \int_{x(z')=x'}^{x(z)=x} \mathcal{D}x \exp\left(-\int_{z'}^z 2k\beta(x, \tilde{z}) \sqrt{1 + \left(\frac{dx}{d\tilde{z}}\right)^2} d\tilde{z}\right) \quad (19)$$

$$= \int_{x(z')=x'}^{x(z)=x} \mathcal{D}x \exp\left(-\int_{z'}^z \mu(x, \tilde{z}) \sqrt{1 + \left(\frac{dx}{d\tilde{z}}\right)^2} d\tilde{z}\right), \quad (20)$$

where $\mu(x, z) = 2k\beta(x, z)$ is the linear attenuation coefficient. 77

3. Propagation using paraxial approximation 78

Consider the propagation of a photon inside a material with a constant refractive index 79 $n_s(x, z) = n_s$. Additionally, assume we are in the near-field regime, where $\frac{dx}{dz}$ is considered 80 to be small, so that: 81

$$\sqrt{1 + \left(\frac{dx}{dz}\right)^2} \approx 1 + \frac{1}{2} \left(\frac{dx}{dz}\right)^2. \quad (21)$$

In consequence, Eq. (11) turns to be:

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$$\begin{aligned} K(x_b, z_b | x_a, z_a) &= \int \mathcal{D}[x(z)] \exp\left(ik \int_{z_a}^{z_b} n_s(x, z) \left[1 + \frac{1}{2} \left(\frac{dx}{dz}\right)^2\right]\right) dz \\ &= \int \mathcal{D}[x(z)] \exp\left(ik n_s \int_{z_a}^{z_b} \left[1 + \frac{1}{2} \left(\frac{dx}{dz}\right)^2\right]\right) dz \\ &= e^{ik(z_b - z_a)} \int \mathcal{D}[x(z)] \exp\left(\frac{ik}{2} n_s \int_{z_a}^{z_b} \left(\frac{dx}{dz}\right)^2\right) dz \end{aligned} \quad (22)$$

The discretized form of the propagator is:

$$\begin{aligned} K(x_b, z_b | x_a, z_a) &= \mathcal{N} e^{ik(z_b - z_a)} \lim_{N \rightarrow \infty} \int dx_{N-1} \cdots \int dx_1 \exp\left(\frac{ik}{2} n_s \sum_{i=1}^N \left(\frac{x_i - x_{i-1}}{\Delta z}\right)^2 \Delta z\right) \\ &= \mathcal{N} e^{ik(z_b - z_a)} \lim_{N \rightarrow \infty} \int dx_{N-1} \cdots \int dx_1 \exp\left(\frac{ik}{2\Delta z} n_s \sum_{i=1}^N (x_i - x_{i-1})^2\right) \\ &= \mathcal{N} e^{ik(z_b - z_a)} \lim_{N \rightarrow \infty} \int dx_{N-1} \cdots \int dx_2 \exp\left(\frac{ik}{2\Delta z} n_s \sum_{i=3}^N (x_i - x_{i-1})^2\right) \\ &\quad \times \int dx_1 \exp\left(\frac{ik}{2\Delta z} n_s [(x_1 - x_0)^2 + (x_2 - x_1)^2]\right), \end{aligned} \quad (23)$$

where $x_0 = x_a$ and $x_N = x_b$. By using the property in Eq. (A3), we can find that:

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$$\begin{aligned}
K(x_b, z_b | x_a, z_a) &= \mathcal{N} e^{ik(z_b - z_a)} \lim_{N \rightarrow \infty} \int dx_{N-1} \cdots \int dx_2 \exp \left(\frac{ik}{2\Delta z} n_s \sum_{i=3}^N (x_i - x_{i-1})^2 \right) \\
&\quad \times \sqrt{\frac{\pi}{-2 \frac{ik}{2\Delta z} n_s}} \exp \left(\frac{\frac{ik}{2\Delta z} n_s}{2} (x_2 - x_0)^2 \right) \\
&= \mathcal{N} e^{ik(z_b - z_a)} \lim_{N \rightarrow \infty} \int dx_{N-1} \cdots \int dx_2 \exp \left(\frac{ik}{2\Delta z} n_s \sum_{i=3}^N (x_i - x_{i-1})^2 \right) \\
&\quad \times \exp \left(\frac{ik}{4\Delta z} n_s (x_2 - x_0)^2 \right) \\
&= \mathcal{N} e^{ik(z_b - z_a)} \lim_{N \rightarrow \infty} \int dx_{N-1} \cdots \int dx_3 \exp \left(\frac{ik}{2\Delta z} n_s \sum_{i=4}^N (x_i - x_{i-1})^2 \right) \\
&\quad \times \int dx_2 \exp \left(\frac{ik}{2\Delta z} n_s (x_3 - x_2)^2 \right) \exp \left(\frac{ik}{4\Delta z} n_s (x_2 - x_0)^2 \right) \\
&= \mathcal{N} e^{ik(z_b - z_a)} \lim_{N \rightarrow \infty} \int dx_{N-1} \cdots \int dx_3 \exp \left(\frac{ik}{2\Delta z} n_s \sum_{i=4}^N (x_i - x_{i-1})^2 \right) \\
&\quad \times \int dx_2 \exp \left(\frac{ik}{4\Delta z} n_s [2(x_3 - x_2)^2 + (x_2 - x_0)^2] \right),
\end{aligned} \tag{24}$$

where the constant $\sqrt{\frac{\pi}{-2 \frac{ik}{2\Delta z} n_s}}$ was absorbed into the normalization constant \mathcal{N} . From now on, all constants from Gaussian integrals will be absorbed into the constant \mathcal{N} . Using the property shown in Eq. (A2), the previous result can be expressed as:

$$\begin{aligned}
K(x_b, z_b | x_a, z_a) &= \mathcal{N} e^{ik(z_b - z_a)} \lim_{N \rightarrow \infty} \int dx_{N-1} \cdots \int dx_3 \exp \left(\frac{ik}{2\Delta z} n_s \sum_{i=4}^N (x_i - x_{i-1})^2 \right) \\
&\quad \times \sqrt{\frac{\pi}{-\frac{3}{4} \frac{ik}{\Delta z} n_s}} \exp \left(\frac{ik}{6\Delta z} n_s (x_3 - x_0)^2 \right) \\
&= \mathcal{N} e^{ik(z_b - z_a)} \lim_{N \rightarrow \infty} \int dx_{N-1} \cdots \int dx_4 \exp \left(\frac{ik}{2\Delta z} n_s \sum_{i=5}^N (x_i - x_{i-1})^2 \right) \\
&\quad \times \int dx_3 \exp \left(\frac{ik}{2\Delta z} n_s (x_4 - x_3)^2 \right) \exp \left(\frac{ik}{6\Delta z} n_s (x_3 - x_0)^2 \right) \\
&= \mathcal{N} e^{ik(z_b - z_a)} \lim_{N \rightarrow \infty} \int dx_{N-1} \cdots \int dx_4 \exp \left(\frac{ik}{2\Delta z} n_s \sum_{i=5}^N (x_i - x_{i-1})^2 \right) \\
&\quad \times \int dx_3 \exp \left(\frac{ik}{6\Delta z} n_s [3(x_4 - x_3)^2 + (x_3 - x_0)^2] \right).
\end{aligned} \tag{25}$$

If we keep using the property shown in Eq. (A2), we can arrive at the next generic expression:

$$\begin{aligned}
K(x_b, z_b | x_a, z_a) &= \mathcal{N} e^{ik(z_b - z_a)} \lim_{N \rightarrow \infty} \int dx_{N-1} \cdots \int dx_{l+1} \exp \left(\frac{ik}{2\Delta z} n_s \sum_{i=\textcolor{red}{l+2}}^N (x_i - x_{i-1})^2 \right) \\
&\times \int dx_{\textcolor{red}{l}} \exp \left(\frac{ik}{2\Delta z} n_s [\textcolor{red}{l}(x_{l+1} - x_l)^2 + (x_l - x_0)^2] \right)
\end{aligned} \tag{26}$$

where l is a fixed index. For $l = N - 2$:

$$\begin{aligned}
K(x_b, z_b | x_a, z_a) &= \mathcal{N} e^{ik(z_b - z_a)} \lim_{N \rightarrow \infty} \int dx_{N-1} \exp \left(\frac{ik}{2\Delta z} n_s \sum_{i=\textcolor{red}{N}}^N (x_i - x_{i-1})^2 \right) \\
&\times \int dx_{\textcolor{red}{N-2}} \exp \left(\frac{ik}{2(N-2)\Delta z} n_s [(\textcolor{red}{N-2})(x_{N-1} - x_{N-2})^2 + (x_{N-2} - x_0)^2] \right) \\
&= \mathcal{N} e^{ik(z_b - z_a)} \lim_{N \rightarrow \infty} \int dx_{N-1} \exp \left(\frac{ik}{2\Delta z} n_s (x_N - x_{N-1})^2 \right) \\
&\times \int dx_{\textcolor{red}{N-2}} \exp \left(\frac{ik}{2(N-2)\Delta z} n_s [(\textcolor{red}{N-2})(x_{N-1} - x_{N-2})^2 + (x_{N-2} - x_0)^2] \right).
\end{aligned} \tag{27}$$

Using property in Eq. (A2) once again:

$$\begin{aligned}
K(x_b, z_b | x_a, z_a) &= \mathcal{N} e^{ik(z_b - z_a)} \lim_{N \rightarrow \infty} \int dx_{N-1} \exp \left(\frac{ik}{2\Delta z} n_s (x_N - x_{N-1})^2 \right) \\
&\times \sqrt{-\frac{\pi}{\frac{N-1}{2(N-2)} \frac{ik}{\Delta z} n_s}} \exp \left(\frac{ik}{2(N-1)\Delta z} n_s (x_{N-1} - x_0)^2 \right) \\
&= \mathcal{N} e^{ik(z_b - z_a)} \lim_{N \rightarrow \infty} \int dx_{N-1} \exp \left(\frac{ik}{2\Delta z} n_s (x_N - x_{N-1})^2 \right) \\
&\times \exp \left(\frac{ik}{2(N-1)} n_s (x_{N-1} - x_0)^2 \right) \\
&= \mathcal{N} e^{ik(z_b - z_a)} \lim_{N \rightarrow \infty} \int dx_{N-1} \exp \left(\frac{ik}{2(N-1)\Delta z} n_s [(N-1)(x_N - x_{N-1})^2 + (x_{N-1} - x_0)^2] \right) \\
&= \mathcal{N} e^{ik(z_b - z_a)} \lim_{N \rightarrow \infty} \sqrt{-\frac{\pi}{\frac{N}{2(N-1)} \frac{ik}{\Delta z} n_s}} \exp \left(\frac{ik}{2N\Delta z} n_s (x_{N-1} - x_0)^2 \right) \\
&= \mathcal{N} e^{ik(z_b - z_a)} \lim_{N \rightarrow \infty} \exp \left(\frac{ik}{2N\Delta z} n_s (x_N - x_0)^2 \right).
\end{aligned} \tag{28}$$

By definition $N\Delta z = z_N - z_0 = z_b - z_a$. Then:

$$K(x_b, z_b | x_a, z_a) = \mathcal{N} e^{ik(z_b - z_a)} \lim_{N \rightarrow \infty} \exp \left(\frac{ik}{2(z_b - z_a)} n_s (x_b - x_a)^2 \right). \tag{29}$$

The expression above no longer depends on N . Then, we can simplify it as:

$$K(x, z|x', z') = \mathcal{N} e^{ik(z-z')} \exp\left(\frac{ik}{2(z-z')} n_s (x-x')^2\right). \quad (30)$$

Since the propagator represents a probability amplitude, it must obey the next normalisation condition:

$$\begin{aligned} 1 &= \left| \int_{-\infty}^{\infty} dx K(x, z|x', z') \right|^2 \\ &= |\mathcal{N}|^2 |e^{ik(z-z')}|^2 \left| \int_{-\infty}^{\infty} dx \exp\left(\frac{ik}{2(z-z')} n_s (x-x')^2\right) \right|^2 \\ &= |\mathcal{N}|^2 \left| \sqrt{-\frac{\pi}{\frac{ik}{2(z-z')} n_s}} \right|^2 \\ &= |\mathcal{N}|^2 \left| \sqrt{\frac{\pi}{\frac{k}{2i(z-z')} n_s}} \right|^2 \\ &\left| \sqrt{\frac{kn_s}{2\pi i(z-z')}} \right|^2 = |\mathcal{N}|^2. \end{aligned} \quad (31)$$

In consequence, we can deduce that:

$$\mathcal{N} = \sqrt{\frac{kn_s}{2\pi i(z-z')}}, \quad (32)$$

and:

$$\begin{aligned} K(x, z|x', z') &= \sqrt{\frac{kn_s}{2\pi i(z-z')}} e^{ik(z-z')} \exp\left(\frac{ikn_s}{2(z-z')} (x-x')^2\right) \\ &= \sqrt{\frac{n_s}{i\lambda(z-z')}} e^{ik(z-z')} \exp\left(\frac{ikn_s}{2(z-z')} (x-x')^2\right), \end{aligned} \quad (33)$$

which corresponds to the 1D Fresnel kernel or 1D Fresnel propagator in real space.

4. Conclusions

Some conclusions here.

Conflicts of Interest

The author declare no conflict of interest.

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Appendix

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A. Gaussian integrals

107

The basic Gaussian integral is given by the next expression: 108

$$\int_{-\infty}^{\infty} dx e^{-a(x-x')^2} = \sqrt{\frac{\pi}{a}}. \quad (\text{A1})$$

An extended version of the basic Gaussian integral, found in the book of Feynman 109
and Hibbs, is given by: 110

$$\int_{-\infty}^{\infty} dx e^{-a(x-x')^2 - b(x''-x)^2} = \sqrt{\frac{\pi}{a+b}} \exp\left(-\frac{(x'-x'')^2}{\frac{1}{a} + \frac{1}{b}}\right). \quad (\text{A2})$$

For $a = b$: 111

$$\int_{-\infty}^{\infty} dx e^{-a((x-x')^2 + (x''-x)^2)} = \sqrt{\frac{\pi}{2a}} \exp\left(-\frac{a}{2}(x'-x'')^2\right) \quad (\text{A3})$$

B. Dirac delta

112

The Dirac delta Fourier-functional form in terms of path integrals is given by: 113

$$\delta[f[x(z)] - g[x(z)]] = \int \mathcal{D}[J[x(z)]] \exp\left(-2\pi i \int dz J[x(z)](f[x(z)] - g[x(z)])\right) \quad (\text{B1})$$

The product of a Dirac delta distribution and a function $f(x)$ is given by: 114

$$f(x)\delta(x-a) = f(a)\delta(x-a) \quad (\text{B2})$$

C. Path Integral for Intensities

115

Taking into account the results in Eqs. (12) and (15), the intensity $I(x, z)$ is given by: 116

$$\begin{aligned}
I(x, z) &= \psi(x, z)\psi^*(x, z) \\
&= \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dx'' \delta(x'' - x') K(x, z|x', z') K^*(x, z|x'', z') \psi(x', z') \psi^*(x'', z') \quad (\text{C1}) \\
&= \int_{-\infty}^{\infty} dx' K(x, z|x', z') K^*(x, z|x', z') I(x', z')
\end{aligned}$$

where $I(x', z') = \psi(x', z')\psi^*(x', z')$, and the Dirac delta term $\delta(x'' - x')$ was included [117](#) to ensure that the paths considered in the path integrals defining $K(x, z|x', z')$ and [118](#) $K(x, z|x'', z')$ begin from the same fixed point. The product of the propagators in Eq. [119](#) ([C1](#)) is: [120](#)

$$\begin{aligned}
K(x, z|x', z') K^*(x, z|x', z') &= \left(\int_{x(z')=x'}^{x(z)=x} \mathcal{D}x e^{iS[x, \frac{dx}{dz}]} \right) \left(\int_{\tilde{x}(z')=x'}^{\tilde{x}(z)=x} \mathcal{D}\tilde{x} e^{-iS^*[\tilde{x}, \frac{d\tilde{x}}{dz}]} \right) \quad (\text{C2}) \\
&= \int_{x(z')=x'}^{x(z)=x} \int_{\tilde{x}(z')=x'}^{\tilde{x}(z)=x} \mathcal{D}x \mathcal{D}\tilde{x} e^{i(S[x, \frac{dx}{dz}] - S^*[\tilde{x}, \frac{d\tilde{x}}{dz}])}
\end{aligned}$$

The initial conditions $x(z') = x'$ and $\tilde{x}(z') = x'$ are assumed to be included in $S[x, \frac{dx}{dz}]$ [121](#) and $S[\tilde{x}, \frac{d\tilde{x}}{dz}]$, respectively. However, the upper limits $x(z) = x$ and $\tilde{x}(z) = x$ can be [122](#) imposed by using Dirac delta functions via: [123](#)

$$K(x, z|x', z') K^*(x, z|x', z') = \int \int \mathcal{D}x \mathcal{D}\tilde{x} \delta(x(z) - x) \delta(\tilde{x}(z) - x) e^{i(S[x, \frac{dx}{dz}] - S^*[\tilde{x}, \frac{d\tilde{x}}{dz}])}. \quad (\text{C3})$$

Using the property [,](#) we can find that: [124](#)

$$\begin{aligned}
K(x, z|x', z') K^*(x, z|x', z') &= \int \int \mathcal{D}x \mathcal{D}\tilde{x} \delta(x(z) - x) \delta(\tilde{x}(z) - x(z)) e^{i(S[x, \frac{dx}{dz}] - S^*[\tilde{x}, \frac{d\tilde{x}}{dz}])} \\
&= \int \mathcal{D}x \delta(x(z) - x) \int \mathcal{D}\tilde{x} \delta(\tilde{x}(z) - x(z)) e^{i(S[x, \frac{dx}{dz}] - S^*[\tilde{x}, \frac{d\tilde{x}}{dz}])} \\
&= \int \mathcal{D}x \delta(x(z) - x) e^{i(S[x, \frac{dx}{dz}] - S^*[x, \frac{dx}{dz}])} \\
&= \int \mathcal{D}x \delta(x(z) - x) e^{-2 \operatorname{Im}(S[x, \frac{dx}{dz}])} \\
&= \int_{x(z')=x'}^{x(z)=x} \mathcal{D}x e^{-2 \operatorname{Im}(S[x, \frac{dx}{dz}])}.
\end{aligned} \quad (\text{C4})$$

In consequence: [125](#)

$$I(x, z) = \int_{-\infty}^{\infty} dx' K_I(x, z|x', z') I(x', z'), \quad (\text{C5})$$

where the term $K_I(x, z|x', z')$ is given by:

$$K_I(x, z|x', z') = \int_{x(z')=x'}^{x(z)=x} \mathcal{D}x e^{-2 \operatorname{Im}(S[x, \frac{dx}{dz}])} \quad (\text{C6})$$

$$I(x_b, z_b | x_a, z_a) = \int_{\substack{x(z_b) = x_b \\ x(z_a) = x_a}} Dx P[x(z)] \subset F_I[x_b, z_b | x_a, z_a]$$

$$= \int_{\mathbb{R}} Dx \delta(x(z_b) - x_b) P[x(z)]$$

Since

$$\delta[f(x) - g(x)] = \int DJ e^{i \int J(x) (f(x) - g(x)) dx}$$

$$\delta[x(t_b) - x_b] = \int DJ e^{i \int J(x) (x(z_b) - x_b)} \quad (J = 2\pi i T)$$

$$= \frac{1}{2\pi i} \int DJ e^{\int J(x) (x(z_b) - x_b)}$$

$$\begin{aligned} \rightarrow I(x_b, z_b | x_a, z_a) &= \frac{1}{2\pi i} \int Dx \int DJ e^{\int J(x) (x(z_b) - x_b)} P[x(z)] \\ &= \frac{1}{2\pi i} \int Dx \int DJ e^{\int J(x) (x(z_b) - x_b + x_a - x_a)} P[x(z)] \\ &= \frac{1}{2\pi i} \int Dx \int DJ e^{\int J(x) (x(z_b) - x_a)} e^{i \int J(x) (x_a - x_b)} P[x(z)] \\ &= \frac{1}{2\pi i} \int Dx \int DJ e^{\int J(x) (x(z_b) - x_a)} e^{-i \int J(x) (x_b - x_a)} P[x(z)] \\ &= \frac{1}{2\pi i} \int DJ e^{-\int J(x) (x_b - x_a)} \int Dx e^{\int J(x) (x(z_b) - x_a)} P[x(z)] \end{aligned}$$

$$= \frac{1}{2\pi i} \int D\zeta e^{-J(x_b - x_a)} Z[J]$$

Where $Z[J] = \int Dx e^{J(x(z_b) - x_a)} P[x(z)]$

$$= \int Dx \sum_{n=0}^{\infty} \frac{1}{n!} (J(x(z_b) - x_a))^n P[x(z)]$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \int Dx J^n (x(z_b) - x_a)^n P[x(z)]$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} J^n \int Dx (x(z_b) - x_a)^n P[x(z)]$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} J^n \langle (x(z_b) - x_a)^n \rangle_{x(z_a)=x_a}$$

$$= 1 + \sum_{n=1}^{\infty} \frac{1}{n!} J^n \langle (x(z_b) - x_a)^n \rangle_{x(z_a)=x_a}$$

Then

$$\begin{aligned} I(x_b, z_b | x_a, z_a) &= \frac{1}{2\pi i} \int D\zeta e^{-J(x_b - x_a)} \left[1 + \sum_{n=1}^{\infty} \frac{1}{n!} J^n \langle (x(z_b) - x_a)^n \rangle \right. \\ &= \frac{1}{2\pi i} \int D\zeta e^{-J(x_b - x_a)} + \frac{1}{2\pi i} \sum_{n=1}^{\infty} \frac{1}{n!} \int D\zeta e^{-J(x_b - x_a)} J^n \langle (x(z_b) - x_a)^n \rangle \\ &= \delta[x_b - x_a] + \frac{1}{2\pi i} \sum_{n=1}^{\infty} \frac{1}{n!} \int D\zeta e^{-J(x_b - x_a)} J^n \langle (x(z_b) - x_a)^n \rangle \\ &= \delta[x_b - x_a] + \frac{1}{2\pi i} \sum_{n=1}^{\infty} \frac{1}{n!} \langle (x(z_b) - x_a)^n \rangle \int D\zeta e^{-J(x_b - x_a)} J^n \end{aligned}$$

$$\text{Let } Z_2 = \int DJ e^{-J(x_b - x_a)} = 2\pi i \delta[x_b - x_a]$$

Then

$$\frac{\partial Z_2}{\partial x_b} = \int DJ (-J) e^{-J(x_b - x_a)} = - \int DJ e^{-J(x_b - x_a)} J$$

$$\frac{\partial^2 Z_2}{\partial x_b^2} = \int DJ e^{-J(x_b - x_a)} J^2$$

$$\Rightarrow \frac{\partial^n Z_2}{\partial x_b^n} = (-1)^n \int DJ e^{-J(x_b - x_a)} J^n$$

$$\Rightarrow \int DJ e^{-J(x_b - x_a)} J^n = (-1)^n \frac{\partial^n Z_2}{\partial x_b^n} = (-1)^n \frac{\partial^n}{\partial x_b^n} 2\pi i \delta[x_b - x_a]$$

$$= 2\pi i \left(-\frac{\partial}{\partial x_b} \right)^n \delta[x_b - x_a]$$

In consequence

$$\begin{aligned} I(x_b, z_b | x_a, z_a) &= \delta[x_b - x_a] + \sum_{n=1}^{\infty} \frac{1}{n!} \langle (x(z_b) - x_a)^n \rangle \left(-\frac{\partial}{\partial x_b} \right)^n \delta[x_b - x_a] \\ &= \delta[x_b - x_a] + \sum_{n=1}^{\infty} \frac{1}{n!} \left(-\frac{\partial}{\partial x_b} \right)^n \left(\langle (x(z_b) - x_a)^n \rangle \delta[x_b - x_a] \right) \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{\partial}{\partial x_b} \right)^n \left(\langle (x(z_b) - x_a)^n \rangle \delta[x_b - x_a] \right) \end{aligned}$$

Evolution eq. tells that:

$$I(x_b, z_b) = \int dx_a I(x_b, z_b | x_a, z_a) I(x_a, z_a)$$

$$\text{Let } x_b = x, z_b = z + \delta z, x_a = x - \delta x, z_a = z$$

$$I(x, z + \delta z) = \int d(\delta x) I(x, z + \delta z | x - \delta x, z) I(x - \delta x, z)$$

$$= \int \frac{d(\delta x)}{n!} \sum_{n=0}^{\infty} \left(-\frac{\partial}{\partial x} \right)^n \left(\langle (x(z + \delta z) - x)^n \rangle \delta[\delta x] \right) I(x - \delta x, z)$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{\partial}{\partial x} \right)^n \langle (x(z + \delta z) - x)^n \rangle I(x, z)$$

$$I(x, z + \delta z) = I(x, z) + \sum_{n=1}^{\infty} \frac{1}{n!} \left(-\frac{\partial}{\partial x} \right)^n \left(\langle (x(z + \delta z) - x)^n \rangle I(x, z) \right)$$

$$\frac{I(x, z + \delta z) - I(x, z)}{\delta z} = \sum_{n=1}^{\infty} \frac{1}{n!} \left(-\frac{\partial}{\partial x} \right)^n \left(\frac{\langle (x(z + \delta z) - x)^n \rangle}{\delta z} I(x, z) \right)$$

$$\text{Let } D_n(x) = \lim_{\delta z \rightarrow 0} \frac{\langle (x(z + \delta z) - x)^n \rangle}{\delta z}, \text{ then, if } \delta z \rightarrow 0:$$

$$\frac{\partial I}{\partial z} = \sum_{n=1}^{\infty} \frac{1}{n!} \left(-\frac{\partial}{\partial x} \right)^n (D_n(x) I(x, z))$$

Let $D_1(x) = \frac{1}{k} \frac{\partial \phi}{\partial x}$ and $D_2(x) = D(x)$:

$$\frac{\partial I}{\partial z} = -\frac{2}{k} \left(\frac{1}{k} \frac{\partial \phi}{\partial x} I(x,z) \right) + \frac{1}{2} \frac{\partial^2}{\partial x^2} (D(x) I(x,z)) + \sum_{n=3}^{\infty} \frac{1}{n!} \left(-\frac{2}{k} \right)^n (D_n(x) I(x,z))$$

X-ray Fokker-Planck eqt.

Consider Langevin eqt!

$$\frac{dx}{dt} = \underbrace{\frac{1}{k} \frac{\partial \phi}{\partial x}}_{F(x)} + \underbrace{\sqrt{D(x)}}_{g(x)} n(t) \quad (n(t) : \text{stochastic term})$$

$$\langle n(t) \rangle = 0 \quad \text{and} \quad \langle n(t) n(t') \rangle = \delta(t-t')$$

$$\Rightarrow dx = f(x) dt + \sqrt{D(x)} dW_t \quad (\text{Ito stochastic diff. eqt})$$

$$x_{i+1} - x_i = f_i(x_i) \delta t + \sqrt{D_i(x_i)} w_i \sqrt{\delta t}$$

Itô discretization

w_i : Discrete random variable

$$\langle w_i \rangle = 0, \langle w_i w_j \rangle = \delta_{ij}$$

Then:

$$D_m = \lim_{\delta t \rightarrow 0} \frac{\langle (x(z+\delta t) - x(z))^m \rangle}{\delta t} = \lim_{\delta t \rightarrow 0} \frac{\langle (f_i(x_i) \delta t + \sqrt{D_i(x_i)} w_i \sqrt{\delta t})^m \rangle}{\delta t}$$

$$D_1 = \lim_{\delta z \rightarrow 0} \left\langle f_i(x_i) \delta z + \underbrace{\sqrt{D_i(x_i)} w_i \sqrt{\delta z}}_{\delta z} \right\rangle = \lim_{\delta z \rightarrow 0} \left\langle f_i(x_i) + \frac{\sqrt{D_i(x_i)} w_i}{\sqrt{\delta z}} \right\rangle$$

$$= f(x) = \frac{1}{k} \frac{\partial \phi}{\partial x}$$

$$D_2 = \lim_{\delta z \rightarrow 0} \frac{\left\langle f_i(x_i) \delta z^2 + D_i(x_i) w_i^2 \delta z + 2f_i(x_i) \sqrt{D_i(x_i)} w_i \delta z \sqrt{\delta z} \right\rangle}{\delta z}$$

$$= \lim_{\delta z \rightarrow 0} \left\langle f_i(x_i) \delta z + D_i(x_i) w_i^2 + 2f_i(x_i) \sqrt{D_i(x_i)} w_i \sqrt{\delta z} \right\rangle$$

$$= D(x)$$

$$D_3 = \lim_{\delta z \rightarrow 0} \frac{\langle O(\delta z^3) \rangle}{\delta z} = \lim_{\delta z \rightarrow 0} \langle O(\delta z) \rangle = 0$$

$$D_n = 0 \quad (n \geq 3) \quad (\text{Pawula's theorem})$$