Consider a parallel-beam tomographic geometry for imaging an object comprising two materials present with atom number density $n_a^{(i)}(x,y,z)$ for i=1,2. This quantity has units of m^{-3} since it is a number density. We illuminate with a spatially uniform incident beam with spectrum $I_{in}^{(j)}(E)$. The superscript j will allow for varying incident spectra. The detector is assumed to detect photons with energy weighting $w^{(j)}(E)$; here the j could allow for different photon counting bins or detector layers in a dual-layer detector. We assume propagation-based phase contrast as derived in Paganin, with detector set a distance Δ behind the sample. According to their derivation starting on page 278, there are four assumptions

- 1. Paraxial and monochromatic (though they later argue polychromatic can be handled; I am going to assume monochromatic in a few steps anyhow)
- 2. Fresnel propagator valid: $\sqrt{k^2 k_x^2 k_y^2} \approx k \frac{\left(k_x^2 + k_y^2\right)}{2k}$
- 3. $\exp\left[\frac{-i\Delta(k_x^2+k_y^2)}{2k}\right] \approx 1 \frac{-i\Delta(k_x^2+k_y^2)}{2k}$
- 4. Intensity in unpropagated field slowly varying in x and y (in going from 4.117 to 4.118).

Then:

 $I_{\Delta}^{(j)}(\xi,\phi,z) = \int dE \, w \, (E) \, I_{in}^{(j)}(E) \, T \, (\xi,\phi,z;E) \left(1 + \frac{\Delta}{k(E)} \nabla^2 \phi \, (\xi,\phi,z;E)\right)$ Here $T \, (\xi,\phi,z;E) = \exp \left[-2r_e \lambda(E) \sum_i A^{(i)} \, (\xi,\phi,z) \, f_2^{(i)}(E)\right]$

is the transmission factor, where r_e is the classical electron radius $(2.8 \times 10^{-15} \text{ m})$, $\lambda(E)$ is the wavelength (given by hc/E, where $hc = 1.24 \times 10^{-9} \text{ m keV}$), $f_2^{(i)}(E)$ is the dimensionless imaginary part of the number of oscillator modes for material i at energy E, and

$$A^{(i)}(\xi,\phi,z) = \int n_a^{(i)}(\xi\cos\phi - \eta\sin\phi, \xi\sin\phi + \eta\cos\phi, z) d\eta$$

$$= RT \text{ for each material}$$

is just the Radon transform through the number density at angular orientation ϕ and radial coordinate ξ . This is done independently at each z.

The phase contribution comes in the final term. Here $k(E) = 2\pi/\lambda(E)$ and

$$\wedge \phi\left(\xi,\phi,z;E\right) = r_e \lambda(E) \sum_i A^{(i)}\left(\xi,\phi,z\right) f_1^{(i)}\left(E\right).$$

The Laplacian $\nabla^2 = \frac{\partial^2}{\partial \xi^2} + \frac{\partial^2}{\partial z^2}$ is applied perpendicular to the propagation direction (i.e., over the ξ , z coordinates of the detector at each angle ϕ).

Let's consider monochromatic illumination at two different energies

$$I_{in}^{(j)}(E) = I_i \delta(E - E_i)$$

and also assume the detector is energy integrating and responds linearly to each photon so $w_j(E) = E$.

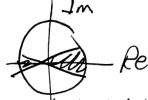
$$I_{\Delta}^{\left(j
ight)}\left(\xi,\phi,z
ight)=E_{j}I_{j}\exp\left[-2r_{e}\lambda_{j}\sum_{i}A^{\left(i
ight)}\left(\xi,\phi,z
ight)f_{2}^{\left(i
ight)}\left(E_{j}
ight)
ight]\left(1+rac{\Delta r_{e}\lambda_{j}}{k_{j}}\sum_{i}
abla^{2}A^{\left(i
ight)}\left(\xi,\phi,z
ight)f_{1}^{\left(i
ight)}\left(E_{j}
ight)
ight),$$

where we have introduced some compact notation like $\lambda_j \equiv \lambda(E_j)$.

The goal is to solve for the two material sinograms $A^{(i)}(\xi,\phi,z)$ given the two intensity measurement sinograms $I_{\Delta}^{(j)}(\xi,\phi,z)$. The questions we are interested in are

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- 1. Does having the phase information help condition his problem? I.e., is there an advantage to $\Delta \neq 0$?
- 2. Is there some optimum Δ ? In varying Δ we need to keep in mind that many of the approximations break down as Δ gets too large.
- 3. Can we compare this to the case where we don't vary spectrum but instead vary the propagation distance Δ ?
- 4. Where exactly do the approximations break down?

Two complications in the above are that the equation is nonlinear in these two unknowns and also that the Laplacian poses challenges. We can use a Rytov-style approximation if $\frac{\Delta r_e \lambda_j}{k_i} \sum_i \nabla^2 A^{(i)}(\xi, \phi, z) f_1^{(i)}(E_j) \ll$ 1. In that case

$$\left(1 + \frac{\Delta r_e \lambda_j}{k_j} \sum_{i} \nabla^2 A^{(i)}\left(\xi, \phi, z\right) f_1^{(i)}\left(E_j\right)\right) \approx \exp\left(\frac{\Delta r_e \lambda_j}{k_j} \sum_{i} \nabla^2 A^{(i)}\left(\xi, \phi, z\right) f_1^{(i)}\left(E_j\right)\right)$$

and we have

$$I_{\Delta}^{\left(j\right)}\left(\xi,\phi,z\right)=E_{j}I_{j}\exp\left[-2r_{e}\lambda_{j}\sum_{i}A^{\left(i\right)}\left(\xi,\phi,z\right)f_{2}^{\left(i\right)}\left(E_{j}\right)+\frac{\Delta r_{e}\lambda_{j}}{k_{j}}\sum_{i}\nabla^{2}A^{\left(i\right)}\left(\xi,\phi,z\right)f_{1}^{\left(i\right)}\left(E_{j}\right)\right].$$

Now we can normalize and take log:

$$p_{\Delta}^{\left(j\right)}\left(\xi,\phi,z\right)\equiv-\ln\left[\frac{I_{\Delta}^{\left(j\right)}\left(\xi,\phi,z\right)}{E_{j}I_{j}}\right]=\left[2r_{e}\lambda_{j}\sum_{i}A^{\left(i\right)}\left(\xi,\phi,z\right)f_{2}^{\left(i\right)}\left(E_{j}\right)-\frac{\Delta r_{e}\lambda_{j}}{k_{j}}\sum_{i}\nabla^{2}A^{\left(i\right)}\left(\xi,\phi,z\right)f_{1}^{\left(i\right)}\left(E_{j}\right)\right].$$

Now take the Fourier transform with respect to ξ and z:

$$P_{\Delta}^{(j)}(k_{\xi},\phi,k_{z}) = 2r_{e}\lambda_{j}\sum_{i}A^{(i)}(k_{\xi},\phi,k_{z})f_{2}^{(i)}(E_{j}) - \frac{\Delta r_{e}\lambda_{j}}{k_{j}}\sum_{i}(k_{\xi}^{2} + k_{z}^{2})A^{(i)}(k_{\xi},\phi,k_{z})f_{1}^{(i)}(E_{j}).$$

This has solved the problem with the differential Laplacian and turned this into an algebraic equation

$$P_{\Delta}^{(j)}(k_{\xi},\phi,k_{z}) = \sum_{i} \left[2r_{e}\lambda_{j} f_{2}^{(i)}(E_{j}) - \left(k_{\xi}^{2} + k_{z}^{2}\right) \frac{\Delta r_{e}\lambda_{j}}{k_{j}} f_{1}^{(i)}(E_{j}) \right] A^{(i)}(k_{\xi},\phi,k_{z}).$$

At each k_{ξ}, ϕ, k_z we have a 2×2 system of equations

$$P_{\Delta}^{(j)}(k_{\xi},\phi,k_{z}) = \sum_{i} H_{ji}(k_{\xi},k_{z})A^{(i)}(k_{\xi},\phi,k_{z}),$$

where

$$H_{ji}(k_{\xi}, k_{z}) = 2r_{e}\lambda_{j} f_{2}^{(i)}(E_{j}) - \left(k_{\xi}^{2} + k_{z}^{2}\right) \frac{\Delta r_{e}\lambda_{j}}{k_{j}} f_{1}^{(i)}(E_{j}).$$

What about the assumptions?

- 1. $\exp\left[\frac{-i\Delta(k_x^2+k_y^2)}{2k}\right] \approx 1 \frac{-i\Delta(k_x^2+k_y^2)}{2k}$ requires that $\frac{\Delta(k_x^2+k_y^2)}{2k} \ll 1$. At 20 keV $\lambda = 6 \times 10^{-11}$ m. So $k \sim 10^{-11}$ 10^{11} . The highest frequencies, if we are well sampled with $\Delta x = 1$ micron are $k_x^{max} = \frac{1}{2\Delta x} = 0.5 \times 10^6$ m^{-1} so $max\left(k_x^2+k_y^2\right)=0.5\times 10^{12}$ and $\frac{\Delta max\left(k_x^2+k_y^2\right)}{2k}=2.5\Delta$ with delta in m. So a 10 cm Δ gives 0.25. Is this \ll 1 enough? Smaller Δ , higher energy, or poorer resolution will make this approximation
- 2. $\frac{\Delta r_e \lambda_i}{k_i} \sum_i \nabla^2 A^{(i)}(\xi, \phi, z) f_1^{(i)}(E_i) \ll 1.$

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