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Taking into account wave effects in Monte Carlo simulation of phase contrast imaging using the Wigner Distribution Function

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X-ray phase contrast imaging (XPCI) is a technique which allows improved image analysis and interpretation by inclusion of phase information alongside absorption. Fig. 1 represents a framework for propagation-based XPCI. Simulation of XPCI permits definition of a precise method aiming for use in various fields.^{1,2} It is by incorporating different phenomena into the frameworks that better understanding can be obtained, this must be done by taking into account both wave and particle-effects. For the moment, artefacts that appear in experimental images, are not obtained during the simulations. A hypothesis is that incoherent scattering in the sample might contribute to noise during the phase retrieval.³⁻⁵ The Wigner Distribution Function (WDF) represents information both on the wave and particle nature of light.⁶ Here we use it to combine both effects within a single framework, and include scattering. Several approaches combining phase contrast and incoherent scattering have recently been proposed. These methods are either two-part simulations or combined methods.⁷⁻¹⁰ Review papers exist.^{5,11,12} We propose a new way to simulate both coherent and incoherent effects using the WDF.

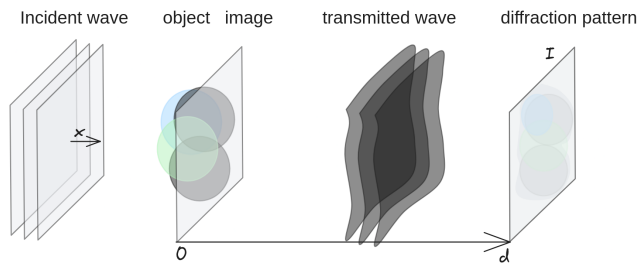


Figure 1: Physical model of propagation-based XPCI: incident plane waves are scattered by an object, this imprints a phase and absorption image on the transmitted wave fronts. The resulting intensity (diffraction pattern) is recorded at some distance behind the object.

The Wigner Distribution Function (WDF) can specifically be applied to optics.¹³ A wave function (Ψ) takes a position (x) and an angle of propagation (θ) for a set of photons, for which the WDF will compute probabilities of their presence at a specific moment of the system. The WDF has the ability to converge to the spectral density function for stationary processes while maintaining full equivalence with the non-stationary autocorrelation function. As a result, it provides a (rough) indication of how the spectral density evolves over time.¹⁴ This is represented as a quasiprobability density (negative particle formulation of quantum physics¹⁵) and as used in our simulation, will *transform* waves to particles by generating particle trajectories.

Cuypers et al.¹⁶ present an analytical solution of the WDF for the double-slit; this enables us to bypass the challenging numerical difficulties associated to the WDF, for this initial demonstration. The presented framework implements the double-slit experiment, through use of the analytical WDF, by calculating the intensities at both the slits and the detector. The photon by photon simulation combines the contributions of coherent diffraction (wave-effect aspect) and incoherent scattering (particle effect). As a first demonstration of the framework, we simulate the double-slit experiment, as well as a variant with a scattering object in one of the slits.

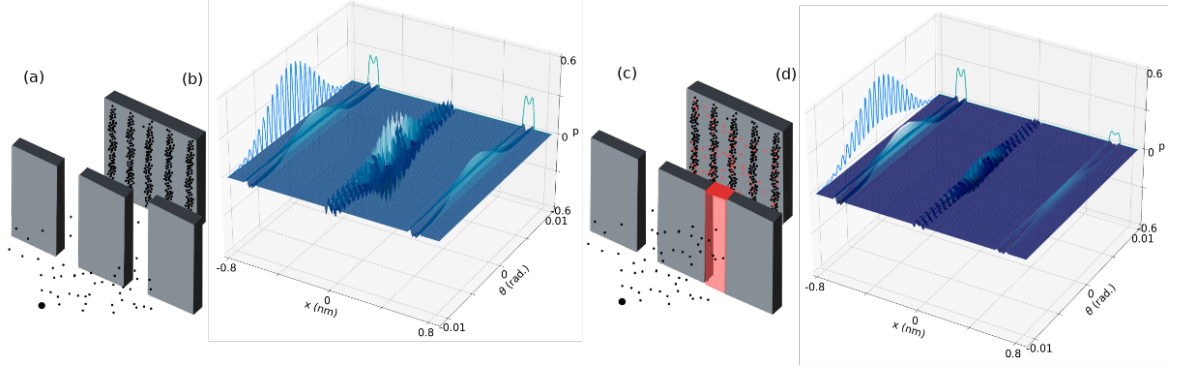


Figure 2: Numerical experiments and their corresponding Wigner distribution function (WDF). (a) The double-slit experiment modelled by the rectangular functions. (b) Analytic WDF and its marginals: intensity in the spatial and angular domains, respectively. (c) Modified double-slit experiment with a scattering element in one of the slits. (d) Corresponding WDF with the amplitude in the slit with the scatterer reduced to 35 %.

The oscillatory nature of the Fourier transform of the rectangular function will impact the analytical WDF, many oscillations are present in the interference term (fig. 2). The projection representing the signal at the exit plane includes oscillations identified as the Gibbs effect, which are not present in the simulations.

These oscillations are somewhat controlled with the parameters used to define the double-slit framework. The number of intensity fringes can be controlled through the slit parameters and the wavelength: slit width is $A = 90$ nm, the slit positions are $a = \pm 600$ nm, and the wavelength is 1 nm corresponding to a photon energy of 1.23 keV. The angular distribution used for the calculation of the spatial probability with interference, and for the simulation is $\theta_{W_f} \in [-0.011, 0.011]$, the spatial distribution is $x \in [-700$ nm, 700 nm]. The detector is fixed at a width of $x \in [-20$ μm , 20 μm].

A proof that this framework is valid, is comparison between the expected intensity distribution and the resulting simulations. Tested along different distances, the method proves to work in both the near- and far-field (3a, 3b). A photon by photon interference pattern can be reconstructed with the framework (3c). Addition of a scattering element is promising, however not realistic for the moment. Proof that a scattering element is successfully simulated is the intensity distribution resembling that of the single slit; the framework promises close results to reproducing this effect.

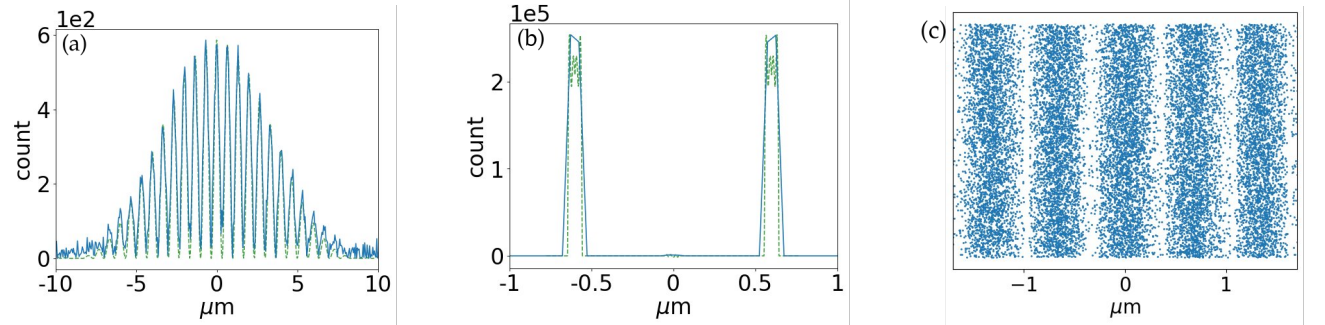


Figure 3: Simulations at different distances with the theoretical double-slit pattern shown in dashed green (a) Comparison between the analytical WDF along the spatial distribution and the simulated result for 1 million photons at $D = 800$ μm (b) Comparison between the analytical WDF along the angular distribution and the simulated result for 1 million photons at $D = 1$ nm (c) Interference fringes for 50 thousand photons at $D = 800$ μm .

A better understanding of the physics behind XPCI will allow step-by-step improvement towards clinical applications.^{17,18} A broader perspective for this application is that it would allow to address the low-frequency noise problem in phase retrieval by providing data for machine learning-based algorithms by simulating scattering and phase contrast.

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