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Diffraction as scattering under the Born approximation

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Abstract: Light diffraction at an aperture is a basic problem that has generated a tremendous amount of interest in optics. Some of the most significant diffraction results are the Fresnel-Kirchhoff and Rayleigh-Sommerfeld formulas. These theories are based on solving the wave equation using Green's theorem and result in slightly different expressions depending on the particular boundary conditions employed. In this paper, we show that the diffraction by a thin screen, which includes apertures, gratings, transparencies etc, can be treated more generally as a particular case of scattering. Furthermore, applying the first order Born approximation to 2D objects, we obtain a general diffraction formula, without angular approximations. Finally, our result, which contains no obliquity factor, is consistent with the 3D theory of scattering. We discuss several common approximations and place our results in the context of existing theories.

According to Born and Wolf, "Diffraction problems are amongst the most difficult ones encountered in optics" [1]. During a period when Newton's corpuscular theory of light [2] was generally accepted, Huygens' incredible intuition provided new insights into the propagation of optical fields [3]. Later on, as Young [4] and Fresnel [5] cemented the wave theory of light, Huygens' principle was placed in a more rigorous mathematical formalism (for a collections of memoirs by Huygens, Young, and Fresnel, one can consult Ref. [6]). Informative reviews in historical context of the scalar diffraction theory can be found in [1] (Chap. VII) and [7] (Chap. 3).

With the advance of quantitative phase imaging (QPI) [8,9], an imaging approach that relies on the refractive index as intrinsic contrast marker, the fields of imaging and angular scattering have been placed in unified physical context as two equivalent descriptions of the same light-tissue interaction [10]. The link between these descriptions is the phase of the optical field, which allows the retrieval of the complex field and numerically express it in either the spatial or wavevector domains. Light scattering models have been paired with phase measurements to reconstruct the 3D structure of cells and tissues, i.e., to solve inverse problems [11–18]. This unified approach of imaging and scattering has been extended to dynamic mass transport in live cells [19–21].

Following this approach of unification of light scattering and imaging, we now propose to extend this common treatment of light scattering and diffraction. Presentation of diffraction as a special case of scattering under the Born approximation can help us solve inverse problems efficiently in the frequency domain. We derive the general formula for the diffracted field generated by an arbitrary incident field at a screen, starting with the inhomogeneous wave equation. As a particular case, we solve the diffraction problem of the spherical wave at an aperture and we express the field without angular approximations. The approach presented here is novel and significant in three major ways, as follows. First, to our knowledge, this is the first time that the diffraction formula was derived from the Born approximation. The closest work to this study is Ref. [22]. which introduces obliquity factor modifications to unify 2D diffraction and 3D scattering problems. However, our mathematical derivation method is different. Second, as described by Goodman (Chapter 3 in [7]), the Rayleigh -Sommerfeld and Kirchhoff theories

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suffer from inconsistencies in the boundary conditions, which result in three different solutions. Our derivation, with no angular approximations, settles this problem and yields a unique solution, with no "obliquity" factor. Third, our work also solves the inconsistency between the Born approximation solutions (see, e.g., Chapter XIII in [1], with no obliquity factor, and diffraction formulas, which contain this factor (Chapter 3 in [7])) as there is no obliquity factor in the 3D scattering solution.

We start with the inhomogeneous Helmholtz equation,

$$[\nabla^2 + \beta^2(\mathbf{r})]U(\mathbf{r};\omega) = 0, \tag{1}$$

where, $\beta(\mathbf{r}) = n(\mathbf{r})\omega/c$ is the wavenumber, with n the inhomogeneous refractive index. Equation (1) can be separated into a homogenous and source term, namely

$$(\nabla^2 + \beta_0^2)U(\mathbf{r};\omega) = -[n^2(\mathbf{r}) - 1]\beta_0^2 U(\mathbf{r};\omega). \tag{2}$$

where, $\beta_0 = {}^{\omega}/_{c}$, is the free space wavenumber.

Figure 1(a) shows the diffraction geometry. We consider the incident field, U_0, impinging on a transparent screen, infinitesimally thin, such that the refractive index distribution can be modelled as (Fig. 1(b))

$$n^2(\mathbf{r}) - 1 = [n^2(\mathbf{r}) - 1]\Pi\left(\frac{z}{\Delta z}\right). \tag{3}$$

where Π is the rectangular function of width Δz, $\Pi(\mathrm{x}) = 1\, for\ x \in [-0.5, 0.5]$ and vanishes outside this range. Here, the suggested slice in Fig. 1(b) is mathematically captured by the rectangular function Π. For an infinitesimally thin object (screen) shown in Fig. 1(b), the scattering potential is proportional to $n^2(\mathbf{r}) - 1 \simeq [n^2(\mathbf{r}_\perp) - 1]\Delta z\delta(z)$, where δ is Dirac's function and $\mathbf{r}_\perp = (x, y)$ the transverse coordinate. We define the transmission function of the diffracting screen to be of the form,

$$t(\mathbf{r}_\perp) = \beta_0[n^2(\mathbf{r}_\perp) - 1]\Delta z. \tag{4}$$

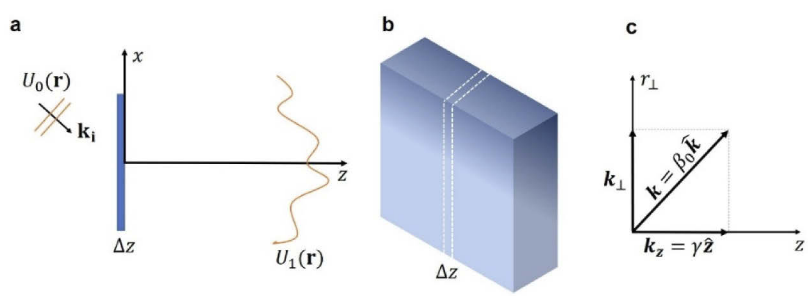

Fig. 1. Diffraction at a thin screen. a. Plane wave, $U_0(\mathbf{r})$, propagating with a wavevector, $\mathbf{k_i}$, is incident on a thin diffracting object. Each point inside the aperture acts as a secondary point source, emitting spherical waves that sum up to form a diffraction pattern at an observation plane. b. The diffracting screen is modelled as a slice of infinitesimal width Δz in the z direction. c. Wavevector, with its transverse and longitudinal component notations, as used in text.

The Helmholtz equation becomes,

$$(\nabla^2 + \beta_0^2)U(\mathbf{r};\omega) = -\beta_0\delta(z)t(\mathbf{r}_\perp)U(\mathbf{r};\omega), \tag{5}$$

The solution of Eq. (5), U, is the sum of the incident field, U_0, and diffracted field, U_1, $U = U_0 + U_1$, with U_0 satisfying the homogenous wave equation. We consider that the thin

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screens involved in common diffraction problems satisfy the first-order Born approximation, which allows us to replace U on the right hand side of Eq. (5) with U_0.

Thus, solving Eq. (5) for U_1 in k-domain, we obtain

$$U_1(\mathbf{k};\omega) = \frac{\beta_0}{k^2 - \beta_0^2}[t(\mathbf{k}_\perp) \circledcirc_{\mathbf{k}} U_0(\mathbf{k};\omega)], \tag{6a}$$

where $\circledcirc_{\mathbf{k}}$ stands for the convolution integral over $\mathbf{k}$ (we use the same notation for a function and its Fourier transform, but carry the arguments explicitly to avoid any confusions). In order to bring the field expression in the $(\mathbf{k}_\perp, z)$ representation, we first separate the k_z-dependence in Eq. (6a) as

$$\begin{aligned} U_1(\mathbf{k};\omega) &= \frac{\beta_0}{k_z^2 - \gamma^2(\mathbf{k}_\perp)}[t(\mathbf{k}_\perp) \circledcirc_{\mathbf{k}} U_0(\mathbf{k};\omega)] \\ &= \frac{\beta_0}{2\gamma(\mathbf{k}_\perp)}\left(\frac{1}{k_z - \gamma(\mathbf{k}_\perp)} - \frac{1}{k_z + \gamma(\mathbf{k}_\perp)}\right)[t(\mathbf{k}_\perp) \circledcirc_{\mathbf{k}} U_0(\mathbf{k};\omega)] \end{aligned}, \tag{6b}$$

where $\gamma^2(\mathbf{k}_\perp) = \beta_0^2 - k_\perp^2$ (see, e.g., [23]).Taking the inverse Fourier Transform with respect to k_z, we use the fact that the term $1/(k^2 - \beta_0^2)$ yields an inverse Fourier Transform for the outgoing wave (neglecting the back propagating wave component) of the form $i\frac{e^{i\gamma(\mathbf{k}_\perp)z}}{2\gamma(\mathbf{k}_\perp)}$, As a result, Eq. (6b) can be re-written as

$$\begin{aligned} U_1(\mathbf{k}_\perp, z;\omega) &= i\frac{\beta_0\, e^{i\gamma(\mathbf{k}_\perp)z}}{2\gamma(\mathbf{k}_\perp)} \circledcirc_z [t(\mathbf{k}_\perp)\delta(z) \circledcirc_{\mathbf{k}_\perp} U_0(\mathbf{k}_\perp, z;\omega)] \\ &= i\frac{\beta_0\, e^{i\gamma(\mathbf{k}_\perp)z}}{2\gamma(\mathbf{k}_\perp)} \circledcirc_z [\delta(z)t(\mathbf{k}_\perp) \circledcirc_{\mathbf{k}_\perp} U_0(\mathbf{k}_\perp, 0;\omega)] \end{aligned}, \tag{7}$$

where we used the property of the delta-function that yields $\delta(z)U_0(\mathbf{k}_\perp, z;\omega) = U_0(\mathbf{k}_\perp, 0;\omega)\delta(z)$.

Finally, using the convolution property of a delta-function [24], Eq. (7) simplifies to

$$U_1(\mathbf{k}_\perp, z;\omega) = i\beta_0\, [t(\mathbf{k}_\perp) \circledcirc_{\mathbf{k}_\perp} U_0(\mathbf{k}_\perp, 0;\omega)]\frac{e^{i\gamma(\mathbf{k}_\perp)z}}{2\gamma(\mathbf{k}_\perp)} \tag{8}$$

Equation (8) represents a very general diffraction formula in the angular spectrum representation, i.e., the $(\mathbf{k}_\perp, z)$ domain, which recovers the well-known result (see, e.g., Ref. 7, Chap. 3, and Fig. 1(c)). This representation exhibits an interesting feature in that the only z-dependence comes from the phase term $e^{i\gamma(\mathbf{k}_\perp)z}$, which makes predicting the diffracted field distribution at various planes $z = z_1, z_2$, etc., particularly easy as we can translate a field from z_1 to z_2 by simply multiplying with $e^{i\gamma(\mathbf{k}_\perp)(z_2 - z_1)}$

Bringing the result into the spatial domain, by taking the inverse Fourier transform of Eq. (8) with respect to $\mathbf{k}_\perp$, we recover the Huygens-Fresnel formula, namely,

$$U_1(\mathbf{r}_\perp, z;\omega) = -i\beta_0 \left[U_0(\mathbf{r}_\perp, 0;\omega)t(\mathbf{r}_\perp) \circledcirc_{\mathbf{r}_\perp} \frac{e^{i\beta_0 r}}{r}\right]. \tag{9}$$

Note that assuming the incident field a plane wave along z, such that $U_0(\mathbf{r};\omega) = A(\omega)e^{ik_{iz}z}$, Eq. (9) becomes $U_1(\mathbf{r}_\perp, z;\omega) = -i\beta_0\, A(\omega)e^{ik_{iz}z}\left[t(\mathbf{r}_\perp) \circledcirc_{\mathbf{r}_\perp} \frac{e^{i\beta_0 r}}{r}\right]$. Various approximation commonly encountered in practice can be obtained easily from Eq. (8) by invoking different degrees of small-angle assumptions (Fig. 2).

First, if we approximate $\gamma \simeq \beta_0$ in the amplitude term of Eq. (8), we obtain,

$$U_1(\mathbf{k}_\perp, z;\omega) \simeq \frac{i}{2}A(\omega)t(\mathbf{k}_\perp)e^{i\gamma(\mathbf{k}_\perp)z}. \tag{10}$$

Equation (10) is the angular spectrum propagation approximation, which simplifies the field propagation significantly. However, Eq. (10) is a fairly accurate representation of the field for most

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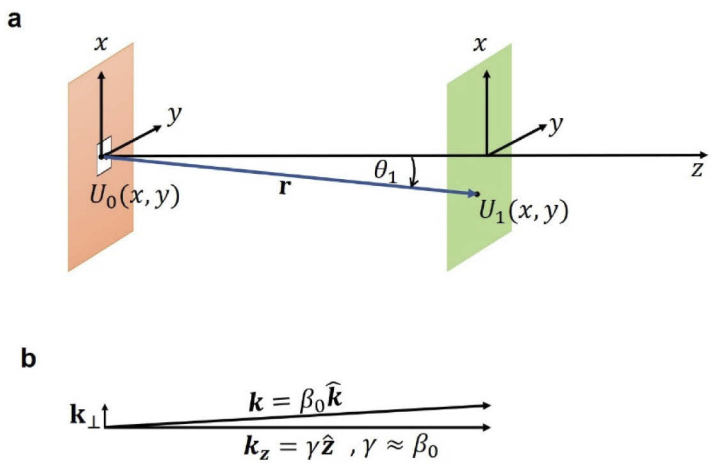

Fig. 2. Approximations. a. Diffracting aperture is placed at z=0 and observation plane is at z. Field at the aperture and observation is U_0(x, y) and U_1(x, y) respectively, **r** is the position vector of the observation point and Θ_1 is the angle of observation. b. For small angle approximations or at sufficiently large distance z, $\gamma \approx \beta_0$.

applications, as it keeps the phase term intact. The next, coarser approximation is due to Fresnel, which is obtained by approximating γ in the phase term as $\gamma \simeq \beta_0 \left(1 - \frac{k_\perp^2}{2\beta_0^2}\right)$. Substituting this in Eq. (10)

$$U_1(\mathbf{k}_\perp, z; \omega) = \frac{i}{2} A(\omega) t(\mathbf{k}_\perp) e^{i\beta_0 \left(1 - \frac{k_\perp^2}{2\beta_0^2}\right) z}. \tag{11}$$

In the spatial domain, the Fresnel approximation gives the well-known result

$$U_1(\mathbf{r}_\perp, z; \omega) = \frac{-i\beta_0}{2z} A(\omega) e^{i\beta_0 z} \left[e^{i\beta_0 \left(\frac{r_\perp^2}{2z}\right)} \circledv_{\mathbf{r}_\perp} t(\mathbf{r}_\perp) \right] \tag{12}$$

Finally, the coarsest approximation is due to Fraunhofer, which, for even smaller angles of diffraction, allows us to neglect quadratic terms in the convolution in Eq. (12). The Fraunhofer approximation yields the diffracted field being expressed as the Fourier transform of the transmission function, namely

$$\begin{aligned} U_1(x, y, z; \omega) &= \tfrac{-i\beta_0}{2z} A(\omega) e^{i\beta_0 z} e^{i\beta_0 \left(\frac{x^2+y^2}{2z}\right)} t(k_x, k_y) \\ k_x &= \beta_0 x/z, \quad k_y = \beta_0 y/z \end{aligned} \tag{13}$$

Next, we apply the Born approximation formalism to the classical problem of the spherical wave diffracting at an aperture (Fig. 3), which was studied by Rayleigh, Fresnel, Kirchhoff and Sommerfeld. In order to solve for the incident field generated by an arbitrary point source at an aperture (Fig. 3), we consider the source as $\delta(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r_0})$, with spectral dependence denoted by $A(\omega)$, driving the wave equation,

$$\nabla^2 U_0(\mathbf{r}) + \beta_0^2 U_0(\mathbf{r}) = A(\omega)\delta(\mathbf{r} - \mathbf{r_0}) \tag{14}$$

In Eq. (14), the field solution, U_0, represents the incident field, which can be used to calculate the diffracted field U_1 via Eq. (8). In the **k** domain, U_0 can be obtained at once,

$$U_0(\mathbf{k}) = \frac{-e^{-i\mathbf{k}.\mathbf{r_0}}}{k^2 - \beta_0^2}, \tag{15a}$$

which in the spatial domain yields a shifted spherical wave,

$$U_0(\mathbf{r}) = \frac{e^{i\beta_0|\mathbf{r}-\mathbf{r_0}|}}{|\mathbf{r}-\mathbf{r_0}|}, \tag{15b}$$

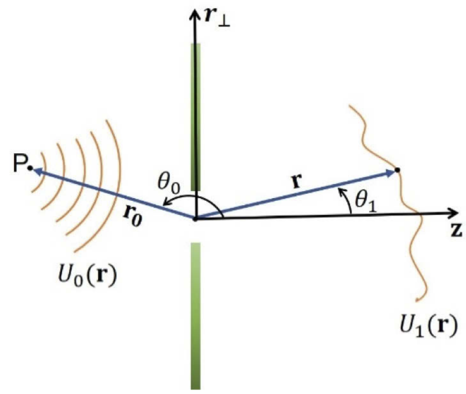

Fig. 3. Diffraction by an aperture. P is the illuminating point source with position vector, $\boldsymbol{r_0}$, making an angle Θ_0 with the outward normal to aperture surface. $U_0(\mathbf{r})$ is the incident field at the aperture and $U_1(\mathbf{r})$ is the diffracted field at observation point with position vector $\mathbf{r}$ making an angle Θ_1 with the outward normal to aperture surface.

Thus, the diffracted field can be obtained using the general solution in Eq. (9), namely,

$$U_1(\mathbf{r}) = -i\beta_0 A(\omega)\iint_a \frac{e^{i\beta_0|(\mathbf{r'}_\perp,0)-\mathbf{r_0}|}}{|(\mathbf{r'}_\perp,0)-\mathbf{r_0}|}\frac{e^{i\beta_0|\mathbf{r}_\perp-\mathbf{r'}_\perp,z|}}{|\mathbf{r}_\perp-\mathbf{r'}_\perp,z|}d^2\mathbf{r'}_\perp \tag{16}$$

Changing the notations (as shown in Fig. 4) to those used in Ref. [7], and using the relationships, $\mathbf{r_0} = (x_2, y_2, z_2)$, $\mathbf{r'} = (x_1, y_1, 0)$, $\mathbf{r'}_\perp = (x_1, y_1)$, $\mathbf{r} = (x_0, y_0, z_0)$, $\mathbf{r}_\perp = (x_0, y_0)$, $r_{21} = \sqrt{(x_2-x_1)^2+(y_2-y_1)^2+{z_2}^2} = |(\mathbf{r'}_\perp,0)-\mathbf{r_0}|$, $r_{01} = \sqrt{(x_0-x_1)^2+(y_0-y_1)^2+{z_0}^2} = |\mathbf{r}_\perp-\mathbf{r'}_\perp,z|$.

Equation (16) transforms to

$$U(x_0,y_0,z_0) = \frac{A(\omega)}{i\lambda}\iint_a \frac{e^{i\beta(r_{21}+r_{01})}}{r_{21}r_{01}}ds \tag{17}$$

which is consistent with conventional diffraction formula as described in Ref. [7] and reiterated in Eq. (18), with obliquity factor $f(\theta)$=1.

$$U(x_0,y_0,z_0) = \frac{A}{i\lambda}\iint_a \frac{e^{i\beta(r_{21}+r_{01})}}{r_{21}r_{01}}f(\theta)ds\ . \tag{18}$$

where, the obliquity factor $f(\theta)$ for the three conventional diffraction solutions are

$$f(\theta) = \begin{cases} \frac{1}{2}[\cos(\mathbf{n},\mathbf{r_{01}}) - \cos(\mathbf{n},\mathbf{r_{21}})] \text{ for Kirchoff} \\ \cos(\mathbf{n},\mathbf{r_{01}}) \text{ for Rayleigh - Sommerfeld - I} \\ -\cos(\mathbf{n},\mathbf{r_{21}}) \text{ for Rayleigh - Sommerfeld - II}\ . \end{cases}$$

A MATLAB simulation of our solution (Eq. (17) and the three conventional diffraction solutions (Eq. (18) for axial intensity calculations based on [25], show that our solution matches closely

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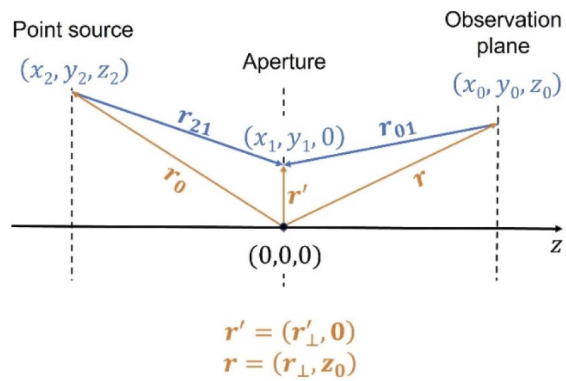

Fig. 4. Notations: In blue, we show the coordinate notations that convert our result into an identical form with that in Ref. [7].

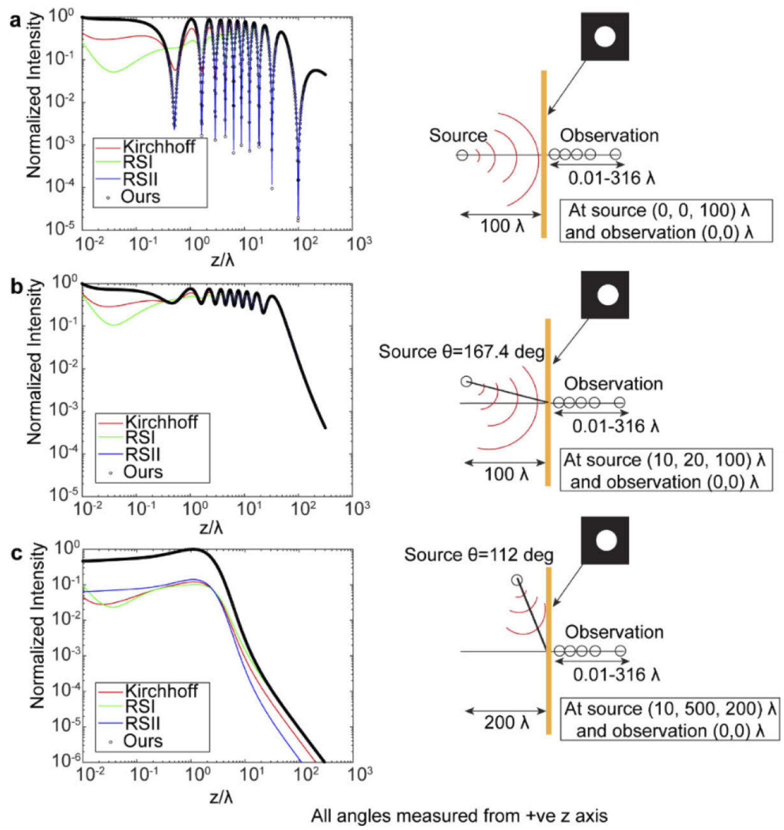

Fig. 5. Comparison of our results with the existing formulas through simulation of diffraction through a circular aperture in an opaque screen illuminated by a diverging point source: a. point source is on axis, our solution matches Rayleigh -Sommerfeld-II solution, b. point source is off-axis at a small angle, our solution still matches Rayleigh -Sommerfeld-II solution, c. point source is off-axis at a large angle, our solution matches the Rayleigh -Sommerfeld-II solution trend (blue line) but is scaled in amplitude.

with Rayleigh-Sommerfeld-II solution when the diverging point source is on axis (Fig. 5(a)) or at a small angle from the axis (Fig. 5(b)). However, as evident in Fig. 5(c), when the angle of illumination increases, our solution while still closely following Rayleigh-Sommerfeld-II solution, gets scaled in magnitude, which is expected due the lack of obliquity factor. As mentioned in [26], for thin phase objects, which is essential to our diffraction formalism presented here, Rayleigh-Sommerfeld-II solution matches well with the experimental results as compared to the other two conventional solutions, validating our approach. We note that the difference between our solution and the three conventional solutions decreases as the propagation distance increases.

In summary, we presented an approach to derive the expression for diffraction by a thin object directly, without the need for a priori boundary conditions. The starting point in this derivation is the realization that scattering and diffraction are fundamentally driven by the same interaction of light with inhomogeneous media. Traditionally, “scattering” refers to interaction with 3D objects, while “diffraction” generally describes the light emerging from 2D objects such as apertures, thin gratings and screens. However, applying the scattering Born approximation to thin 3D objects, we showed that the general formulation for diffraction can be obtained without angular approximations. Our result is consistent with the three classical formulas described in Ref. [7] with unit obliquity factor. As pointed out in Ref. [22], obliquity factor can be reintroduced if we modify the Green’s function through a mathematical adjustment, which, as per the paper itself, has no realistic physical explanation. However, an aim of our study is to avoid any such mathematical assumptions which have no physical explanations and hence demonstrate a simple way to reach the diffraction formulas through scattering.

Traditionally, the field of light imaging, diffraction, and Fourier Optics, have been mainly concerned with the 2D problem and captured mostly an engineering audience. On the other hand, light scattering, dealing with the 3D interaction, seems to be mostly driven by physicists. We hope that revisiting this classical problem with a unifying formalism of scattering and diffraction may help bring closer the fields of optical imaging and scattering, which are in essence different descriptions on the same light-matter interaction phenomenon.

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Data Availability. No data was generated in this study.

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