Physical Light-Matter Interaction in Hermite-Gauss Space — Supplemental and Derivations

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In this supplemental manuscript, we derive the relevant properties of the anisotropic Hermite-Gauss, prove the primary theoretical Lemmas that appear in the paper and discuss polarization as well as the Wigner-Ville distribution in Hermite-Gauss space.

S1 THE ANISOTROPIC HERMITE-GAUSS FUNCTIONS

The (univariate) Hermite-Gauss functions are defined as follows:

$$\Psi_n(x) \triangleq \left(\sqrt{\pi}2^n n!\right)^{-1/2} \mathrm{e}^{-\frac{x^2}{2}} H_n(x) = \frac{(-1)^n \mathrm{e}^{\frac{x^2}{2}}}{\sqrt{\sqrt{\pi}2^n n!}} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \mathrm{e}^{-x^2}, \quad \text{(S1.1)}$$

for $x \in \mathbb{R}$, with integer $n \geq 0$ being the degree and H_n the Hermite polynomials. These functions are known to form an orthogonal and complete basis of scalar L^2 functions [Szegö 1939] and to be the eigenfunctions of the Fourier transform with the associated eigenvalues being $\sqrt{2\pi}(-\mathrm{i})^n$, viz. $\mathscr{F}\left\{\Psi_n\right\} = \sqrt{2\pi}(-\mathrm{i})^n \Psi_n$ [Wiener 1988].

The anisotropic HG functions were defined in Eq. (5), and we also write the generating functions of the HG functions and their dual functions [Takemura and Takeuchi 1988]:

$$\sum_{n,m,l} \frac{2^{\frac{n+m+l}{2}}}{\sqrt{n!m!l!}} \alpha_x^n \alpha_y^m \alpha_z^l \Psi^{\Theta}_{nml}(\vec{r}) = \frac{\mathrm{e}^{-\frac{1}{2}\vec{r}^\top\Theta^{-1}\vec{r}+\vec{\alpha}^\top\Theta^{-1}(2\vec{r}-\vec{\alpha})}}{\left(\pi^3|\Theta|\right)^{\frac{1}{4}}}, \quad \text{(S1.2)}$$

$$\sum_{n,m,l} \frac{2^{\frac{n+m+l}{2}}}{\sqrt{n!m!l!}} \alpha_x^n \alpha_y^m \alpha_z^l \widetilde{\Psi}^{\Theta}_{nml}(\vec{r}) = \frac{\mathrm{e}^{-\frac{1}{2}\vec{r}^\top\Theta^{-1}\vec{r}+\vec{\alpha}^\top(2\vec{r}-\Theta\vec{\alpha})}}{\left(\pi^3|\Theta|\right)^{\frac{1}{4}}}, \quad \text{(S1.3)}$$

which holds for any $\vec{r}, \vec{\alpha} \in \mathbb{R}^3$. We now discuss some properties of the anisotropic HG functions.

Orthogonality and completeness. The anisotropic Hermite-Gauss functions are mutually orthogonal with respect to their dual function, viz.

$$\left\langle \Psi^{\Theta}_{nml} \middle| \widetilde{\Psi}^{\Theta}_{n'm'l'} \right\rangle = \delta_{nn'}\,\delta_{mm'}\,\delta_{ll'}, \quad \text{(S1.4)}$$

as well as complete, i.e. if $\forall n,m,l,\ \langle \Psi^{\Theta}_{nml} \mid f \rangle = 0$ for some function f, then $f \equiv 0$. See Takemura and Takeuchi [1988] for a proof of orthogonality. Proof of completeness follows the univariate case (see Hochstadt [1986]).

Fourier transform of the HG functions. To study the Fourier transform of the anisotropic HG functions, we begin with the generating function (Eq. (S1.2)), take the FT of both sides and perform the variable changes $\vec{\beta} = \Theta^{-1/2}\vec{\alpha}$ and $\vec{s}' = \Theta^{-1/2}\vec{r}'$, hence $\mathrm{d}\vec{r}' = |\Theta|^{1/2}\mathrm{d}\vec{s}'$ (as $|\Theta|^{1/2}$ is the Jacobian), in the FT integral, viz.

$$\begin{aligned}
&\sum_{n,m,l} \frac{2^{\frac{n+m+l}{2}}}{\sqrt{n!m!l!}} \alpha_x^n \alpha_y^m \alpha_z^l \mathscr{F}\left\{\Psi^{\Theta}_{nml}(\vec{r}')\right\}(\vec{\zeta}) \\
&= \left(\pi^{-3}|\Theta|\right)^{\frac{1}{4}} \mathscr{F}\left\{\mathrm{e}^{-\frac{1}{2}(s')^2+2\vec{\beta}\cdot\vec{s}'-\beta^2}\right\}\left(\sqrt{\Theta}^\top\vec{\zeta}\right) \\
&= \left(2\sqrt{\pi}\right)^{\frac{3}{2}} |\Theta|^{\frac{1}{4}} \mathrm{e}^{-\frac{1}{2}\vec{\zeta}^\top\Theta\vec{\zeta}+2(-\mathrm{i}\vec{\alpha})\cdot\vec{\zeta}+(-\mathrm{i}\vec{\alpha})^\top\Theta^{-1}(-\mathrm{i}\vec{\alpha})} \\
&= (2\pi)^{\frac{3}{2}} \sum_{n,m,l} \frac{2^{\frac{n+m+l}{2}}}{\sqrt{n!m!l!}} (-\mathrm{i})^{n+m+l} \alpha_x^n \alpha_y^m \alpha_z^l \widetilde{\Psi}^{\Theta^{-1}}_{nml}\left(\vec{\zeta}\right),
\end{aligned} \quad \text{(S1.5)}$$

where in the last step we applied the generating function of the dual HG function identity (Eq. (S1.3)). Equating the powers of $\vec{\alpha}$ on both sides above yields the final result:

$$\mathscr{F}\left\{\Psi^{\Theta}_{nml}(\vec{r}')\right\}(\vec{\zeta}) = (2\pi)^{\frac{3}{2}}(-\mathrm{i})^{n+m+l}\,\widetilde{\Psi}^{\Theta^{-1}}_{nml}\left(\vec{\zeta}\right). \quad \text{(S1.6)}$$

Thus, the anisotropic HG functions and their dual serve as Fourier-transform pairs. We may also conclude that $\Psi^{\boldsymbol{I}}_{nml}$ are the eigenfunctions of the three-dimensional FT, with associated eigenvalues $(2\pi)^{3/2}(-\mathrm{i})^{n+m+l}$. We believe the result above is novel.

Special values of the Hermite-Gauss functions. We state, without proving, a closed-form expression for the anisotropic HG functions evaluated at 0:

$$\Psi^{\Theta}_{nml}(0) = \frac{\sqrt{n!m!l!}}{\left(\pi^3|\Theta|\right)^{\frac{1}{4}}} \sum_{\substack{\boldsymbol{T}\in\mathbb{N}^{3\times3} \\ \text{s.t. } \tau_{1,2,3}\in 2\mathbb{N} \\ [\,1,1,1\,]\boldsymbol{T}=[\,n,m,l\,]^\top}} \left(\prod_{i,j} \frac{q_{ij}^{T_{ij}}}{T_{ij}!}\right) \prod_{l\in\{1,2,3\}} \frac{(\tau_l-1)!_{(2)}}{\mathrm{i}^{\tau_l}} \quad \text{(S1.7)}$$

where $\Theta^{-1/2} = [q]_{ij}$, $[\,\tau_1,\tau_2,\tau_3\,]^\top = \boldsymbol{T}[\,1,1,1\,]^\top$, i.e the row sums of $\boldsymbol{T}$, and $!_{(2)}$ denotes the double factorial. Note that the summation is over 3×3 matrices with natural integer elements, such that the columns are integer partitions of n, m, l and the row sums are even.

Also, directly from the generating function we immediately derive the following identity:

$$\Psi^{\Theta}_{nml}(-\vec{r}) = (-1)^{n+m+l}\,\Psi^{\Theta}_{nml}(\vec{r}). \quad \text{(S1.8)}$$

S2 DERIVATIONS

In this section we perform the derivations of Theorem 3.1 and Lemmas 4.3 and 4.4 in the paper.

S2.1 Scattering and Diffraction

We formulate our theory of light-matter interaction under the scalar diffraction theory, formally formulated via the Huygens-Fresnel

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principle, as follows [Goodman 2017]:

$$u(\vec{r}) = \frac{1}{\mathrm{i}\lambda} |\hat{r} \cdot \hat{n}| \int_{\mathcal{X}} \mathrm{d}^2 \vec{p}'\, u'(\vec{p}') \frac{1}{|\vec{r} - \vec{p}'|} \mathrm{e}^{\mathrm{i}k|\vec{r}-\vec{p}'|} , \tag{S2.1}$$

which is a diffraction integral over some planar aperture $\mathcal{X} \subset \mathbb{R}^3$. u' quantifies the (local) electromagnetic excitations on that aperture and $\hat{n}$ is the aperture's normal (u, u' are treated as deterministic quantities in this context). This integral should be understood as a superposition of spherical waves that originate from every point on the aperture, and it is implied that $r \gg \lambda$. See Fig. 3 for an illustration of the geometry.

Diffraction by planar apertures is of limited interest to applications in the realm of computer graphics. More practical is a discussion of interaction of light with matter: surfaces and participating media. To that end, we proceed in a similar manner to Born and Wolf [1999] to extend the planar aperture $\mathcal{X}$ to a scattering volume: We make the Born first-order approximation, where the electromagnetic field driving the scattering process inside the volume is the incident field only. From a physical perspective, this assumption implies that secondary scattering of the scattered field can be neglected, i.e. the volume scatters weakly with respect to its spatial extent. For example: if the scattering medium is a metal surface, then the Born first-order approximation can be understood as neglecting multiple-scattering by the surface (steep incident and exitance angles are thus ignored); or, if we deal with a participating medium, like a liquid, then we assume that the (secondary) interactions of the scattered field with the medium may be neglected.

Nevertheless, it is important to remember that we deal with partially-coherent light. Hence, the scattering regions are small, with characteristics lengths on the orders of hundreds of micrometres. Repeated interactions between such small, distinct subregions of a scattering medium (for example, path tracing through a dense liquid) are possible under our assumptions.

Under the Born first-order approximation, an incident field induces electromagnetic excitations inside a region in a scattering medium, giving rise to scattered fields. The amplitudes of the scattered fields are quantified by a *scattering amplitude function*, denoted $\sigma(\hat{s}', \hat{r}' ; \vec{p}')$, which describes the amplitude ratio of the scattered wave in direction $\hat{r}'$, produced due to a scattering event in position $\vec{p}'$ in the medium and under excitation by an incident wave from direction $\hat{s}'$. The scattering amplitude function is, in general, wavelength dependant and can take complex values, quantifying the phase-shifts induced by interaction with conducting particles. We are now ready to formulate a more general diffraction integral:

$$u(\vec{r}) = \frac{1}{\mathrm{i}\lambda} \int_{\mathbb{R}^3} \mathrm{d}^3 \vec{p}'\, u'(\vec{r}') \sigma(\hat{s}', \hat{r}' ; \vec{p}') \frac{1}{|\vec{r} - \vec{p}'|} \mathrm{e}^{\mathrm{i}k|\vec{r}-\vec{p}'|} , \tag{S2.2}$$

where $\hat{r}'$ and $\hat{s}'$ are the directions from the integration point $\vec{p}'$ to the observation point $\vec{r}$ and the source $\vec{s}$, respectively. Note that the scattering amplitude function implicitly limits the integration to the spatial extent of the scattering region.

Eq. (S2.2) should be understood as a generalization of Eq. (S2.1) that is able to describe diffraction by apertures and optical elements, as well as scattering by surfaces and by inhomogeneous participating media. The driving assumptions are (i) that the scattering is dominated by *Rayleigh scatterers*, i.e. where the scattered waves are of the same frequency as the incident wave—a good approximation to virtually all non-fluorescent objects [Born and Wolf 1999]; and, (ii) the Born first-order approximation.

Cross-spectral density of the diffracted radiation. We turn our attention to studying the CSD of the diffracted radiation and make the usual Fraunhofer (optical far field) region approximation, implying that the characteristic length of that scattering region is small with respect to the distances to $\vec{r}$ (the observation point) and $\vec{s}$ (the radiation source that gives rise to u'). Let a scattering region (assumed to be centred around the origin) be described via a scattering amplitude function σ, and C' be the CSD of the radiation incident to the scattering region from direction $\hat{s}$. Under the Born first-order approximation and in the Fraunhofer region, the scattered CSD becomes

$$C\left(\vec{r} ; \vec{\xi}_1, \vec{\xi}_2 ; \omega\right) = \frac{\mathrm{e}^{\mathrm{i}k\hat{r}\cdot\left(\vec{\xi}_1-\vec{\xi}_2\right)}}{\lambda^2 r^2} \mathscr{A}\left\{\Sigma \cdot C'\right\}\left(k\hat{r} + \tfrac{k}{r}\vec{\xi}_1, k\hat{r} + \tfrac{k}{r}\vec{\xi}_2\right), \tag{S2.3}$$

where $\mathscr{A}$ is the angular correlation transform operator (Eq. (3)) and we define $\Sigma(\vec{\xi}_1, \vec{\xi}_2) = \sigma(\vec{\xi}_1)\sigma^\star(\vec{\xi}_2)$ as the *scattering mutual intensity.* The integration of the ACT above is done over the variables $\vec{\xi}_{1,2}$ of Σ and C'.

Proof. Starting with Eq. (S2.2), we proceed in a fashion identical to the typical Fourier optics derivation of Fraunhofer region diffraction [Goodman 2017]: In the denominator we may readily approximate $r \approx |\vec{r} - \vec{p}'|$, while a more accurate approximation is needed in the complex exponent and we power expand via the square root's power series, viz. $\sqrt{1+a} = 1 + \frac{1}{2}a + O(a^2)$, yielding

$$|\vec{r} - \vec{p}'| \approx r - \hat{r} \cdot \vec{p}' . \tag{S2.4}$$

Furthermore, we also assume that the scattering amplitude function σ is a slow function of the directions $\hat{s}', \hat{r}'$, and thus approximate $\hat{s}' \approx \hat{s}$ and $\hat{r}' \approx \hat{r}$, i.e. the directions are held constant inside the scattering region. This assumption holds well in the far field when σ does not contain very sharp impulses, as would arise by a Dirac delta reflector (such as a perfect mirror). We discuss how to handle such matter in the paper.

Then, apply the approximations discussed above to Eq. (S2.2) and substitute the resulting expression for the field u into the definition of the CSD (Eq. (10)), yielding the Fourier optics relation quantified in Eq. (S2.3). □

S2.2 Derivation of Lemma 4.3

Start with plugging Definition 4.1 into Eq. (S2.3) and simplifying, which immediately gives rise to the following relation between the incident and scattered beams:

$$\sum_{n,m} \check{c}_{nm}\, \Psi^{\Theta}_{nm}\left(kQ\frac{\vec{\xi}}{r}\right) = \frac{1}{s^2\lambda^2} \sum_{n',m'} \check{c}'_{n'm'} \times \mathscr{A}\left\{\Sigma \cdot \Psi^{\Theta'}_{n'm'}\left(kQ'\frac{\vec{r}'_1-\vec{r}'_2}{s}\right)\right\}\left(\vec{\phi} + \tfrac{k\vec{\xi}}{2r}, \vec{\phi} - \tfrac{k\vec{\xi}}{2r}\right), \tag{S2.5}$$

where $\vec{r}'_{1,2}$ are the ACT integration variables, $\check{c}_{nm}$, Θ are the HG transverse modes and shape matrices, respectively (primed values correspond to the incident CSD and unprimed values to the scattered

CSD), also defined is the shorthand $\vec{\boldsymbol{\phi}} = k(\hat{\boldsymbol{r}} + \hat{\boldsymbol{s}})$ and recall that the orthogonal matrices $\boldsymbol{Q}, \boldsymbol{Q}'$ transform to the local frame of the scattered and incident radiation, respectively.

With Eq. (S2.5) as the starting point, we would like to derive an expression for the coefficients $\check{c}_{nm}$. To isolate each coefficient on the left-hand side in Eq. (S2.5), we take the inner product of both sides with the dual HG function $\widetilde{\Psi}^{\Theta}_{nm}(k\boldsymbol{Q}\frac{\vec{\xi}}{r})$. The left-hand side becomes

$$\sum_{q,p} \check{c}_{qp} \left\langle \Psi^{\Theta}_{qp}\left(k\boldsymbol{Q}\frac{\vec{\xi}'}{r}\right) \middle| \widetilde{\Psi}^{\Theta}_{nm}\left(k\boldsymbol{Q}\frac{\vec{\xi}'}{r}\right) \right\rangle = \sum_{q,p} \check{c}_{qp} \left(\frac{r}{k}\right)^3 \left\langle \Psi^{\Theta}_{qp}\left(\vec{\xi}''\right) \middle| \widetilde{\Psi}^{\Theta}_{nm}\left(\vec{\xi}''\right) \right\rangle = \left(\frac{r}{k}\right)^3 \check{c}_{nm} \,, \quad \text{(S2.6)}$$

where we first did the variable change $\vec{\xi}'' = k\boldsymbol{Q}\frac{\vec{\xi}'}{r}$ in the inner product, the Jacobian is then $|\frac{r}{k}\boldsymbol{Q}^{-1}| = (\frac{r}{k})^3$ (recall $\boldsymbol{Q}$ is orthogonal) and thus $\mathrm{d}^3\vec{\xi}' = (\frac{r}{k})^3\,\mathrm{d}^3\vec{\xi}''$. Finally we applied the orthonormality of the HG function w.r.t. its dual, viz. Eq. (S1.4).

The primary difficulty in the analysis of the right-hand side of Eq. (S2.5) lies in ACT that appears there, and, for brevity, we denote that ACT as $\mathscr{f}_{n'm'}$, i.e.:

$$\mathscr{f}_{n'm'}\left(\vec{\xi}\right) \triangleq \mathscr{A}\left\{\Sigma \cdot \Psi^{\Theta'}_{n'm'}\left(k\boldsymbol{Q}'\frac{\vec{r}_1' - \vec{r}_2'}{s}\right)\right\}\left(\vec{\boldsymbol{\phi}} + \frac{k\vec{\xi}}{2r}, \vec{\boldsymbol{\phi}} - \frac{k\vec{\xi}}{2r}\right) . \quad \text{(S2.7)}$$

Consider the inner product of that ACT with the same dual HG function $\widetilde{\Psi}^{\Theta}_{nm}(k\boldsymbol{Q}\frac{\vec{\xi}}{r})$. By formally interchanging the orders of integrations (i.e., inner product with the ACT), we first take the inner product of the ACT kernel (see the definition, Eq. (3)) with the dual HG function, which is a simple FT. The integration then immediately follows via a variable change as before, the definition of the dual HG function (Eq. (6)) and an application of the FT of the HG function identity (Eq. (S1.6)), viz.

$$\left\langle \mathrm{e}^{-\mathrm{i}\frac{k}{r}\vec{\xi}'\cdot\frac{\vec{r}_1+\vec{r}_2}{2}} \middle| \widetilde{\Psi}^{\Theta}_{nm}\left(\frac{k}{r}\boldsymbol{Q}\vec{\xi}'\right) \right\rangle = \left(\frac{r}{k}\right)^3 (2\pi)^{\frac{3}{2}} (-\mathrm{i})^{m+n}\, \Psi^{\Theta^{-1}}_{nm}\left(\boldsymbol{Q}\frac{\vec{r}_1+\vec{r}_2}{2}\right) . \quad \text{(S2.8)}$$

We are now ready to take the inner product of the right-hand side of Eq. (S2.5) with the dual HG function (with the added factor of $(\frac{k}{r})^3$ that normalises Eq. (S2.6)—the left-hand side), then formally interchange the orders of integrations, apply Eq. (S2.8) and simplify, yielding the transverse HG coefficient:

$$\begin{aligned}
\check{c}_{nm} &= \left(\frac{k}{r}\right)^3 \left\langle \frac{1}{s^2\lambda^2} \sum_{n',m'} \check{c}'_{n'm'} \mathscr{f}_{n'm'}\left(\vec{\xi}'\right) \middle| \widetilde{\Psi}^{\Theta}_{nm}\left(\frac{k}{r}\boldsymbol{Q}\vec{\xi}'\right) \right\rangle \\
&= \frac{(2\pi)^{\frac{3}{2}}(-\mathrm{i})^{n+m}}{s^2\lambda^2} \sum_{n',m'} \check{c}'_{n'm'} \\
&\quad \times \mathscr{A}\left\{\Sigma \cdot \Psi^{\Theta^{-1}}_{nm}\left(\boldsymbol{Q}\frac{\vec{r}_1+\vec{r}_2}{2}\right) \Psi^{\Theta'}_{n'm'}\left(k\boldsymbol{Q}'\frac{\vec{r}_1'-\vec{r}_2'}{s}\right)\right\}\left(\vec{\boldsymbol{\phi}}, \vec{\boldsymbol{\phi}}\right) , \quad \text{(S2.9)}
\end{aligned}$$

with $\vec{r}'_{1,2}$ being the ACT integration variables, proving Lemma 4.3.

S2.3 Derivation of Lemma 4.4

As previously mentioned, the anisotropic HG functions form a complete functional basis, irregardless of the choice for Θ. Hence, Lemma 4.3 gives rise to an underdetermined system: we are free to select the shape matrix as we wish (as long as it remains positive-definite), and Lemma 4.3 would still hold.

As with any underdetermined system, to solve the system and make mathematical progress we need to add additional constraints to the system. To that end, we now consider only the 0^{th}-order HG transverse mode (the mode that corresponds to Ψ^{Θ}_{00}). This is not merely a simplification: Of the main purposes of the shape matrix is to increase the expressiveness of the expansion when using a limited number of modes (otherwise, it would not be needed). The more HG modes we use, the less dependant is the expansion accuracy on Θ. Therefore, we constrain the system to the most restrictive setting—only the lowest-order mode—in order to derive a formula for the shape matrix. Anyhow, the formulae remain mathematically exact.

Under the setting discussed above Lemma 4.4 is derived: Denote $\vec{\boldsymbol{w}} = \frac{k}{r}\vec{\xi}$ and, as before, $\mathscr{f}_{n'm'}(\vec{\boldsymbol{w}})$ (Eq. (S2.7)) as the ACT that appears in Eq. (S2.5). The 0^{th}-order HG function is simply the Gaussian

$$\Psi^{\Theta}_{00}\left(\vec{\boldsymbol{r}}\right) \equiv \frac{1}{\pi^{\frac{3}{4}}|\Theta|^{\frac{1}{4}}} \mathrm{e}^{-\frac{1}{2}\vec{\boldsymbol{r}}^{\intercal}\Theta^{-1}\vec{\boldsymbol{r}}} . \quad \text{(S2.10)}$$

Then, Eq. (S2.5) simplifies to

$$\mathrm{e}^{-\frac{1}{2}\vec{\boldsymbol{w}}^{\intercal}\boldsymbol{Q}^{\intercal}\Theta^{-1}\boldsymbol{Q}\vec{\boldsymbol{w}}} = \frac{\left(\pi^3|\Theta|\right)^{1/4}}{s^2\lambda^2} \frac{\check{c}'_{00}}{\check{c}_{00}} \mathscr{f}_{00}(\vec{\boldsymbol{w}}) . \quad \text{(S2.11)}$$

As discussed in the paper, the even-ordered HG transverse modes are real, therefore all the terms above are real. This also implies that the shape matrix Θ is real, as desired, as well as the function $\mathscr{f}_{00}$—which also follows from the fact that the transformed function in Eq. (S2.7) is symmetric. Then, take the 2^{nd}-order derivative with respect to $\vec{\boldsymbol{w}}$ (i.e., the Hessian) of the natural logarithm of both sides above, yielding:

$$\boldsymbol{Q}\Theta^{-1}\boldsymbol{Q}^{\intercal} = -\frac{\partial^2}{\partial\vec{\boldsymbol{w}}^2} \ln\left[\frac{\left(\pi^3|\Theta|\right)^{1/4}}{s^2\lambda^2} \frac{\check{c}'_{00}}{\check{c}_{00}} \mathscr{f}_{00}\right] . \quad \text{(S2.12)}$$

Using the fact that $\ln(x_1x_2) = \ln(x_1) + \ln(x_2)$, those constant terms above vanish under derivation, therefore Eq. (S2.12) reduces to the interesting relation that constitutes Lemma 4.4, viz.

$$\Theta = -\boldsymbol{Q}^{\intercal}\left[\frac{\partial^2}{\partial\vec{\boldsymbol{w}}^2} \ln \mathscr{f}_{00}(\vec{\boldsymbol{w}})\right]^{-1}_{\vec{\boldsymbol{w}}=0} \boldsymbol{Q} , \quad \text{(S2.13)}$$

with the 0^{th}-th order scattering mode $\mathscr{f}_{00}$ as defined in Eq. (S2.7).

As an aside, observe that the evaluation at $\vec{\boldsymbol{w}} = 0$ above can also be understood simply as the Fraunhofer region condition because clearly $\lim_{r\to\infty}\vec{\boldsymbol{w}} = 0$.

S2.4 Computing the shape matrix

We briefly discuss how to compute the shape matrix via Theorem 5.1.(ii) in the paper (i.e., Eq. (S2.13)).

The following few Lemmas may be of use to make analytic progress towards a Shape matrix once an analytic expression for σ is known. The first one is derived using elementary means:

LEMMA S2.1. *Given f, a twice continuously differentiable function, the following holds:*

$$\frac{\mathrm{d}^2}{\mathrm{d}\vec{r}^2}\ln f = \frac{1}{f}\frac{\mathrm{d}^2}{\mathrm{d}\vec{r}^2}f - \frac{1}{f^2}\nabla f \nabla f^\intercal ,$$

where $\nabla f = \mathrm{d}f/\mathrm{d}\vec{r}$ is the gradient.

The next is a well-known result in linear algebra.

LEMMA S2.2 (RECURSIVE INVERSE OF MATRIX SUM). *Let $\boldsymbol{A}$ be a non-singular $d \times d$ matrix and $\boldsymbol{B} = \boldsymbol{B}_1 + \boldsymbol{B}_2 + \ldots + \boldsymbol{B}_p$ a non-singular matrix with each $\boldsymbol{B}_j$ being a rank-1 matrix. For each $1 \leq j \leq p$, denote $\boldsymbol{C}_j \triangleq \boldsymbol{A} + \boldsymbol{B}_1 + \boldsymbol{B}_2 + \ldots + \boldsymbol{B}_{j-1}$. If all $\boldsymbol{C}_j$ are invertible as well, then,*

$$\boldsymbol{C}_{q+1}^{-1} = \boldsymbol{C}_q^{-1} - t_q \boldsymbol{C}_q^{-1}\boldsymbol{B}_q\boldsymbol{C}_q^{-1} ,$$

with $1 \leq q < p$ and $t_q \triangleq \left[1 + \mathrm{tr}\left(\boldsymbol{C}_q^{-1}\boldsymbol{B}_q\right)\right]^{-1}$. Furthermore,

$$(\boldsymbol{A}+\boldsymbol{B})^{-1} = \boldsymbol{C}_p^{-1} - t_p \boldsymbol{C}_p^{-1}\boldsymbol{B}_p\boldsymbol{C}_p^{-1} .$$

PROOF. See Miller [1981]. □

Consider a twice continuously differentiable, but otherwise arbitrary, function f. Denote

$$\boldsymbol{A} \triangleq \frac{1}{f}\frac{\mathrm{d}^2}{\mathrm{d}\vec{r}^2}f , \tag{S2.14}$$

$$\boldsymbol{B}_1 \triangleq -\frac{1}{f^2}\nabla f \nabla f^\intercal , \tag{S2.15}$$

with $\boldsymbol{B}_1$ clearly being a rank-1 matrix. Then, applying Lemma S2.1 and Lemma S2.2:

$$\left[\frac{\partial^2}{\partial\vec{r}^2}\ln f\right]^{-1} = (\boldsymbol{A}+\boldsymbol{B}_1)^{-1} = \boldsymbol{A}^{-1} - t_1\boldsymbol{A}^{-1}\boldsymbol{B}_1\boldsymbol{A}^{-1} , \tag{S2.16}$$

with

$$t_1 = \left[1 + \mathrm{tr}\left(\boldsymbol{A}^{-1}\boldsymbol{B}_1\right)\right]^{-1} = \left[1 - \frac{1}{f}\mathrm{tr}\left(\nabla f \nabla f^\intercal \frac{\mathrm{d}^2}{\mathrm{d}\vec{r}^2}f\right)\right]^{-1} . \tag{S2.17}$$

Eq. (S2.16) is a closed-form expression that may be useful in computing the shape matrix. The remaining (potentially) involved analytic step is only the computation of $\boldsymbol{A}^{-1}$, which amounts to the inverse Hessian of angular coherence function.

S3 THE WIGNER-VILLE SPECTRUM IN HERMITE-GAUSS SPACE

The *Wigner-Ville Distribution* (WVD) is a powerful bilinear representation of a signal that commonly arise in optics and quantum mechanics, useful for processing linear frequency-modulated signals. It is also commonly know as the *wigner distribution function* and has seen some usage in computer graphics (see Section 2 in the paper), chiefly as a form of a "generalized radiance" (introduced by Walther [1968]), because it remains constant on far-field propagation along a ray from the radiating source—like the classical radiance. This is theoretically pleasant, but serves little practical value because the same couple of problems that we set out to solve in this paper afflict the WVD just as the CSD: it is still a (potentially arbitrary) function, and representing it non-symbolically in a renderer is not straightforward; and, formulation of light-matter interaction remains equally difficult with the WVD, as the a similar diffraction problem to Theorem 3.1 still needs to be solved. Additional shortcomings are noted by Steinberg and Yan [2021b]: it is a less intuitive representation of the important characteristics of the wave ensemble and admits less relevant literature.

In this section we formally show that, in HG space, the WVD and the CSD are intrinsically related. Given a stochastic process with its CSD $C(\vec{r}\,;\vec{\xi}_1,\vec{\xi}_2)$—as in Eq. (10), with the dependence on the angular frequency neglected—the WVD can be formally defined as the directional power spectrum [Born and Wolf 1999]:

$$\mathscr{W}\left(\vec{r}\,;\vec{\zeta}\right) \triangleq \int_{\hat{\boldsymbol{r}}^\perp} \mathrm{d}^2\vec{\xi}^\perp\, C\left(\vec{r}\,;\frac{1}{2}\vec{\xi}^\perp,-\frac{1}{2}\vec{\xi}^\perp\right)\mathrm{e}^{-\mathrm{i}\vec{\zeta}\cdot\vec{\xi}^\perp} , \tag{S3.1}$$

which is a Fourier transform of the CSD evaluated at a separation of $\vec{\xi}^\perp$ over the transverse plane $\hat{\boldsymbol{r}}^\perp$. That transverse plane is centred around the origin, such that $\hat{\boldsymbol{r}}^\perp = \{\vec{\xi}^\perp : \hat{\boldsymbol{r}}\cdot\vec{\xi}^\perp = 0\}$. We reiterate our definition of the far field CSD in Hermite-Gauss space (Definition 4.1), viz.

$$C\left(\vec{r}\,;\vec{\xi}\right) \triangleq \frac{\mathrm{e}^{\mathrm{i}k\hat{\boldsymbol{r}}\cdot\vec{\xi}}}{r^2}\sum_{n,m}\check{c}_{nm}\,\Psi_{nm}^{\Theta}\left(\tfrac{k}{r}\boldsymbol{Q}\vec{\xi}\right) , \tag{S3.2}$$

with some orthogonal $\boldsymbol{Q}$ and recall that $\vec{\xi} = \vec{\xi}_1 - \vec{\xi}_2$, by definition. Applying Eq. (S3.1) to the CSD in HG space above, noting that $\hat{\boldsymbol{r}}\cdot\vec{\xi}^\perp = 0$ and performing the variable change $\vec{\xi}'' = \frac{k}{r}\boldsymbol{Q}\vec{\xi}^\perp$, with the Jacobian being $|\frac{r}{k}\boldsymbol{Q}^{-1}| = (\frac{r}{k})^2$, yields

$$\begin{aligned}\mathscr{W}\left(\vec{r}\,;\vec{\zeta}\right) &= \frac{1}{r^2}\sum_{n,m}\check{c}_{nm}\mathscr{F}\left\{\mathrm{e}^{\mathrm{i}k\hat{\boldsymbol{r}}\cdot\vec{\xi}^\perp}\,\Psi_{nm}^{\Theta}\left(\tfrac{k}{r}\boldsymbol{Q}\vec{\xi}^\perp\right)\right\}\left(\vec{\zeta}\right)\\ &= \frac{1}{k^2}\sum_{n,m}\check{c}_{nm}\mathscr{F}\left\{\Psi_{nm}^{\Theta}\left(\vec{\xi}''\right)\right\}\left(\tfrac{r}{k}\boldsymbol{Q}\vec{\zeta}\right)\\ &= \frac{2\pi}{k^2}\sum_{n,m}(-\mathrm{i})^{n+m}\check{c}_{nm}\,\widetilde{\Psi}_{nm}^{\Theta^{-1}}\left(\tfrac{r}{k}\boldsymbol{Q}\vec{\zeta}\right) ,\end{aligned} \tag{S3.3}$$

where we applied the FT of the Hermite-Gauss function identity (Eq. (S1.6)) at the last step.

Eq. (S3.3) demonstrates that the WVD of a wave ensemble, in HG space, is similar to the representation of the CSD, up to the duality of the HG functions and constants. The close relationship between the CSD and WVD in Hermite-Gauss space suggests that the decision of whether to use the CSD or WVD to quantify a wave ensemble is a matter of preference, and our theory could easily be adapted to a WVD-centric formulation.

Properties of the WVD.

(1) (REALNESS) In the paper, Section 4, we have shown that the odd-ordered HG coefficients correspond to evanescent waves that vanish in the far field. Therefore, $n + m$ is even and $\mathscr{W}$ is real, as expected [Bastiaans 1986].
(2) (SPECTRAL INTENSITY) Applying the inverse Fourier transform to the definition of the WVD, Eq. (S3.1), as well as Eq. (11) yields

$$I(\vec{r}) = C\left(\vec{r}\,;0\right) = \int_{\hat{\boldsymbol{r}}^\perp}\mathrm{d}^2\vec{\zeta}^\perp\,\mathscr{W}\left(\hat{\boldsymbol{r}}\,;r\vec{\zeta}^\perp\right) , \tag{S3.4}$$

which is the observed (positional) spectral intensity, as quantified by the WVD. Recall that we omit the angular frequency from the parameter lists, for brevity.

(3) (Perfectly-incoherent radiation) Hypothetical, perfectly-incoherent radiation could be described via a CSD proportional to a Dirac delta, viz. $C \propto \delta^2(\vec{\xi}^{\perp})$. Then, the WVD takes the form of a function that does not dependent on $\vec{\zeta}$.

(4) (Perfectly-coherent radiation) Conversely, radiation that remains coherent throughout all space admits a CSD that is constant in $\vec{\xi}^{\perp}$, therefore the corresponding WVD takes the form of a Dirac delta in $\vec{\zeta}$.

The first pair of properties above suggest that the quantity

$$\mathscr{W}\left(\hat{\boldsymbol{r}}\,;k\vec{\zeta}\right) = \frac{2\pi}{k^2}\sum_{n,m}(-\mathrm{i})^{n+m}\check{c}_{nm}\,\widetilde{\Psi}_{nm}^{\Theta^{-1}}\left(Q\vec{\zeta}\right) \tag{S3.5}$$

can be understood as a "generalized radiance", that remains constant on free-space propagation, admits some convenient analytic properties and is very closely related to our far-field CSD.

S4 POLARIZATION - GENERALIZED STOKES PARAMETERS

In this section we briefly outline how to incorporate polarization into our formalism, and by doing so show that our theory is consistent with classical electromagnetism. We also introduce the useful *generalized Stoked parameters* to the computer graphics community. This section builds upon the cross-spectral density matrix (sometimes known as the coherency matrix), which we will shortly introduce. See the supplemental material of Steinberg and Yan [2021b] for identities relevant to general polarization matrices. Also see Goodman [2015]; Wolf [2007] for additional information.

In the paper, in Subsection 3.2, we introduced a scalar-valued stochastic process $u(\vec{r},t)$ that describes a wave ensemble, and defined its (scalar) CSD C (Eq. (10)). Electromagnetic fields are vector fields, and we now change the notation: Let $\vec{E}(\vec{r},t)$ be the stochastic process that quantifies the radiation's electric field distribution throughout spacetime (the previous, scalar quantity u can be understood as the magnitude of that field, viz. $u = |\vec{E}|$). Let $\hat{\boldsymbol{k}}$ be the direction of propagation at some point $\vec{r}$, and denote an *orthonormal transverse basis* as the set $\{\hat{\boldsymbol{e}}_1, \hat{\boldsymbol{e}}_2\}$ of vectors that together with $\hat{\boldsymbol{k}}$ form an orthonormal basis. $\vec{E}$ can now be decomposed into its transverse oscillations $E_{1,2} = \hat{\boldsymbol{e}}_{1,2} \cdot \vec{E}$. See Fig. 1. The *cross-spectral density matrix* (CSDM) generalizes the CSD to vector fields: by considering the cross-correlation between these transverse components, the CSDM is defined as:

$$\overleftrightarrow{C}\left(\vec{r}\,;\vec{\xi}_1,\vec{\xi}_2\,;\omega\right) \triangleq \begin{bmatrix} \left\langle E_1(\vec{r}_1)E_1^{\star}(\vec{r}_2)\right\rangle_\omega & \left\langle E_1(\vec{r}_1)E_2^{\star}(\vec{r}_2)\right\rangle_\omega \\ \left\langle E_2(\vec{r}_1)E_1^{\star}(\vec{r}_2)\right\rangle_\omega & \left\langle E_2(\vec{r}_1)E_2^{\star}(\vec{r}_2)\right\rangle_\omega \end{bmatrix} \tag{S4.1}$$

(up to an irrelevant normalization constant) with the shorthands $\vec{r}_{1,2} = \vec{r} + \vec{\xi}_{1,2}$ and $\langle\cdot\rangle_\omega$ being the same ensemble-averaging operator that was defined in the paper (see Eq. (10)), i.e., the ensemble-average over the statistical ensemble of same-frequency realizations of $\vec{E}$. The above matrix is also sometimes known, confusingly, as the "coherence matrix", but this term is also used for non-coherence-aware polarization matrices and should be avoided.

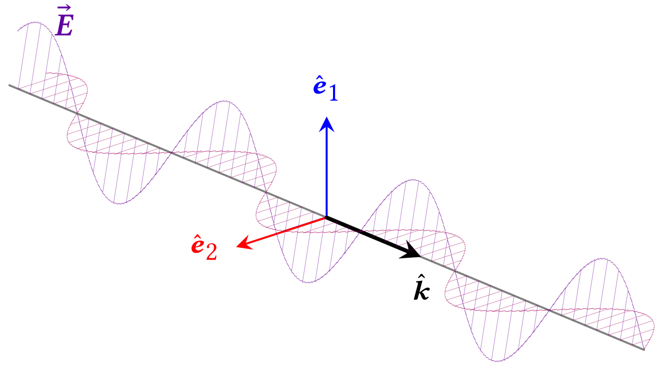

Fig. 1. An electric field $\vec{E}$ decomposed into its transverse components along $\hat{\boldsymbol{e}}_1$ and $\hat{\boldsymbol{e}}_2$, that span the *transverse plane*, which is perpendicular to the direction of propagation $\hat{\boldsymbol{k}}$.

It is easy to see that when $\vec{\xi}_1 = \vec{\xi}_2$, this matrix must be Hermitian (viz. $\overleftrightarrow{C}^{\dagger} = \overleftrightarrow{C}$) and positive semi-definite. Additionally, we state without proving that the observed spectral intensity of the radiation is

$$I(\vec{r}\,;\omega) \triangleq \operatorname{tr}\overleftrightarrow{C}\,(\vec{r}\,;0,0\,;\omega)\,, \tag{S4.2}$$

in stark similarity to the scalar case (Eq. (11) in the paper) and where tr is the matrix trace operator. The complex spectral *degree-of-coherence* is then

$$\gamma\left(\vec{r}\,;\vec{\xi}_1,\vec{\xi}_2\,;\omega\right) \triangleq \frac{\operatorname{tr}\overleftrightarrow{C}\left(\vec{r}\,;\vec{\xi}_1,\vec{\xi}_2\,;\omega\right)}{\sqrt{I\left(\vec{r}+\vec{\xi}_1\,;\omega\right)}\sqrt{I\left(\vec{r}+\vec{\xi}_2\,;\omega\right)}}\,. \tag{S4.3}$$

The complex degree-of-coherence quantifies how coherent the radiation is, with $0 \le |\gamma| \le 1$ (strictly speaking, $|\gamma| = 0$ is aphysical). Finally, the spectral *degree-of-polarization* quantifies how polarized the radiation is (but does not immediately describe which type of polarization arises):

$$\wp(\vec{r}\,;\omega) \triangleq \sqrt{1 - 4\left|\overleftrightarrow{C}\right|\left(\operatorname{tr}\overleftrightarrow{C}\right)^{-2}}\,, \tag{S4.4}$$

where $|\overleftrightarrow{C}|$ denotes the determinant and it is implied that $\vec{\xi}_{1,2} = 0$. For proofs see Steinberg and Yan [2021b, supplemental].

The formulation briefly outlined above describes a unified formalism of coherence and polarization. It is well-known that these concepts are intrinsically related, e.g., the coherence properties of a beam may induce polarization changes on free-space propagation. Moreover, both polarization and coherence affect (and, in-turn, are affected by) the physical process of light-matter interaction. This formalism remains physically accurate as long as the spectral intensity can be recovered from the CSDM via Eq. (S4.2), which is the exact same validity domain that was discussed in the paper (Subsection 3.2) for the scalar case: ergodicity or sufficiently polychromatic radiation. We will now discuss how our theory light-matter interaction works with the CSDM.

S4.1 The Generalized Stokes Parameters

Let the (normalized) Pauli spin matrices be defined as (usually these are denoted as $\boldsymbol{\sigma}_j$, however that notation would clash with the scattering amplitude function)

$$\boldsymbol{\tau}_0 = \frac{1}{2}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}, \qquad \boldsymbol{\tau}_1 = \frac{1}{2}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix},$$
$$\boldsymbol{\tau}_2 = \frac{1}{2}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}, \qquad \boldsymbol{\tau}_3 = \frac{1}{2}\begin{bmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{bmatrix}. \tag{S4.5}$$

The CSDM is Hermitian when evaluated at $\vec{\xi}_1 = \vec{\xi}_2$, therefore we will use these Pauli matrices, which clearly form a basis of the real vector space over 2×2 Hermitian matrices, to decompose the CSDM as follows:

$$\overleftrightarrow{C} = C_0\,\boldsymbol{\tau}_0 + C_1\,\boldsymbol{\tau}_1 + C_2\,\boldsymbol{\tau}_2 + C_3\,\boldsymbol{\tau}_3, \tag{S4.6}$$

where C_j is the coefficient of the j-th matrix in Eq. (S4.5). Each such C_j is a scalar function of $\vec{r}, \vec{\xi}_1, \vec{\xi}_2, \omega$, and together these coefficients form the *generalized Stokes parameters*, introduced by Korotkova and Wolf [2005] (note wrong sign in their Eq. 10c). To ensure Hermiticity, C_j must be real when $\vec{\xi}_1 = \vec{\xi}_2$, otherwise they can take complex values. The coefficients must also fulfil the Poincaré sphere condition $\sqrt{|C_1|^2 + |C_2|^2 + |C_3|^2} \leq |C_0|$.

Using Eq. (S4.6) we can immediately rewrite the quantities that characterize the coherence properties of the wave ensemble using the generalized Stokes parameters:

$$I(\vec{r}\,;\omega) \triangleq C_0\left(\vec{r}\,; 0, 0\,;\omega\right), \tag{S4.7}$$

$$\gamma\left(\vec{r}\,;\vec{\xi}_1,\vec{\xi}_2\,;\omega\right) \triangleq \frac{C_0\left(\vec{r}\,;\vec{\xi}_1,\vec{\xi}_2\,;\omega\right)}{\sqrt{I\left(\vec{r}+\vec{\xi}_1\,;\omega\right)}\sqrt{I\left(\vec{r}+\vec{\xi}_2\,;\omega\right)}}. \tag{S4.8}$$

The immediate conclusion is that the 0^{th} generalized Stokes parameter, C_0, fully describes the spectral intensity carried by the wave ensemble, as well as its coherence properties. The other coefficients describe the polarization properties. The *degree of cross-polarization* takes the convenient form:

$$\mathscr{P}\left(\vec{r}\,;\vec{\xi}_1,\vec{\xi}_2\,;\omega\right) \triangleq \frac{1}{C_0^2}\sqrt{C_1^2+C_2^2+C_3^2}, \tag{S4.9}$$

which reduces to the degree-of-polarization $\wp$ (Eq. (S4.4)) when $\vec{\xi}_{1,2} = 0$. Additional parameters quantify the beam's polarization ellipse. The *semi-axis magnitudes* of the polarization ellipse are [Korotkova 2017]

$$\varsigma_{1,2}(\vec{r}\,;\omega) \triangleq C_3^{-\frac{1}{2}}\left[C_0 \pm \sqrt{C_1^2+C_2^2}\right]^{\frac{1}{2}} \tag{S4.10}$$

and its *spectral orientation angle* is [Korotkova 2017]

$$\psi(\vec{r}\,;\omega) \triangleq \frac{1}{2}\arctan\left(\frac{C_2}{C_1}\right). \tag{S4.11}$$

The spectral orientation angle defines the angle between the first transverse direction $\hat{\boldsymbol{e}}_1$ and the major semi-axis of the polarization ellipse.

It should be remembered that, just as with the coherence matrix $\overleftrightarrow{C}$, the generalized Stokes parameters are defined with respect to the choice of the transverse basis $\hat{\boldsymbol{e}}_{1,2}$. This dependence is implicit and is omitted from the notation.

The reader might note the profound similarities between the discussion above and the classical Stokes parameters, which have been used for polarization-aware radiometric renderers (e.g., [Jarabo and Arellano 2017]). Indeed, the generalized Stokes parameters are to the classical Stokes parameters the same as the CSD is to the classical radiance: we imbue the radiometric radiance with a two-point formalism that allows quantifying the correlation between the waveforms that constitute the statistical ensemble of waves. Therefore, the coefficients of the generalized Stokes parameters describe the polarization state of the radiation in an identical manner to the classical Stokes parameters. Furthermore, when $\vec{\xi}_1 = \vec{\xi}_2$, as discussed the C_j must be real, and indeed they simply reduce to the classical, single-point radiometric Stokes parameters.

S4.2 Light-matter interaction

To apply our theory to the vectorized formalism of polarization and coherence, we use the generalized Stokes parameters C_j, expanded in HG space, in place of the CSD C. The generalized Stokes parameter in HG space takes an identical form to Definition 4.1. Therefore, a wave ensemble is now parametrized by four (instead of one) series of HG coefficients, $\check{c}_{nm}^{(j)}$, expanding the generalized Stokes parameters C_j in HG space, as well as the shape matrix $\boldsymbol{\Theta}$ as before. Note that a single shape matrix is sufficient: C_0 quantifies the coherence properties of the radiation.

The scattering properties of locally-stationary matter need now to be specified via 16 scattering amplitude functions $\sigma^{(j\to l)}(\hat{\boldsymbol{s}}', \hat{\boldsymbol{r}}'\,;\vec{r}')$, which quantifies the matter response in terms of the scattered l-th generalized Stokes parameter, with respect to incident j-th generalized Stokes parameter. The scattering angular coherence $\tilde{f}_\sigma^{(j\to l)}$ and stationary autocorrelation $R_{\sigma\sigma}^{(j\to l)}$ for each scattering amplitude are defined in an identical manner to before, see Eqs. (12) and (13). In this case, Theorem 5.1 in the paper can be rewritten as

Theorem S4.1. *(Polarization-aware interaction of light with locally-stationary matter in HG space). Let $\check{c}_{n'm'}^{\prime(j)}$ and $\boldsymbol{\Theta}'$ be the incident radiation's HG transverse modes for each generalized Stoke parameter and the shape matrix, respectively. Then,*

(i) the scattered HG transverse modes of each generalized Stoke parameter are:

$$\check{c}_{nm}^{(l)} = \sum_{j=0}^{3}\left\langle \tilde{f}_\sigma^{\;(j\to l)} \,\middle|\, \widetilde{\Psi}_{nm}^{\boldsymbol{\Theta}}\left(\boldsymbol{Q}\vec{r}'\right)\right\rangle \times \sum_{n',m'} \frac{1}{s^2\lambda^2}\check{c}_{n'm'}^{\prime(j)}\mathscr{F}\left\{R_{\sigma\sigma}^{(j\to l)}\,\Psi_{n'm'}^{\boldsymbol{\Theta}'}\left(\frac{k\boldsymbol{Q}'\vec{r}'}{s}\right)\right\}\left(\vec{\boldsymbol{\phi}}\right),$$

(ii) and, the shape matrix is:

$$\boldsymbol{\Theta} = \boldsymbol{Q}^\intercal \cdot \left[\frac{\partial^2}{\partial\vec{\zeta}^2}\ln\left|\tilde{f}_\sigma^{\;(0\to 0)}\right|\right]_{\vec{\zeta}=0}^{-1} \cdot \boldsymbol{Q},$$

where $\tilde{f}_\sigma^{(j\to l)}$ and $R_{\sigma\sigma}^{(j\to l)}$ are the matter's scattering angular coherence and stationary autocorrelation functions, respectively.

Note that the formula for the shape matrix only makes use of the $0 \to 0$ scattering mode, as discussed. The equations above retain the same form as in the case of the scalar CSD (Theorem 5.1 in the paper), and all of the results and examples we explored in the paper (in Subsection 5.1) apply to Theorem S4.1 as well. Therefore, the theory is virtually unchanged while the computational requirements are increased up to 16-fold (just as with introducing the Stokes parameters to a radiometric renderer). Though, in practice, usually much of the cross-component scattering (i.e. the $\sigma^{(j\to l)}$ with $j \neq l$) vanishes.

S4.3 ABCD Optical Systems

A large body of optical work has discussed quantifying the effects of an optical element on radiation via a matrix that acts upon the CSDM (which, in the past, was often termed the "coherence matrix" in that literature). This gives rise to a linear formalism, and optical elements that are described using this formulation are sometimes known as "ABCD optical systems". This subsection serves as a very brief overview.

Formally, given some optical element, let $\boldsymbol{T}(\vec{r}\,;\omega)$ be a complex-valued, 2×2 matrix, which should be understood as the *Jones matrix* that describes the *behaviour of the optical element upon a single realization of wave ensemble*, of angular frequency ω, that interacts with the optical element at position $\vec{r}$. Then, the CSDM of the entire ensemble after interactions is given by:

$$\overleftrightarrow{C}\left(\vec{r}\,;\vec{\xi}_1,\vec{\xi}_2\right) = \left\langle \boldsymbol{T}\left(\vec{r}+\vec{\xi}_1\right)\overleftrightarrow{C}'\left(\vec{r}\,;\vec{\xi}_1,\vec{\xi}_2\right)\boldsymbol{T}^\dagger\left(\vec{r}+\vec{\xi}_2\right)\right\rangle\ , \quad \text{(S4.12)}$$

where $\overleftrightarrow{C}'$ is the CSDM of the incident radiation. We drop the ω from the arguments for brevity. Clearly, when $\vec{\xi}_1=\vec{\xi}_2$, Hermiticity and positive semi-definiteness are preserved. This formulation is similar to the Jones calculus discussed by Steinberg and Yan [2021b].

Note that due to the ensemble-average that appears in Eq. (S4.12), the calculus briefly outlined in this subsection is able to describe optical elements that mutate both the coherence and the polarization properties of an incident light beam. This is in contrast to the standard Jones calculus that is capable of neither, and works with fully-coherent, full-polarized beams. It is then easy to show that this calculus is theoretically able to describe arbitrary optical elements. Given fixed $\vec{r}$, $\vec{\xi}_{1,2}$ and ω, 16 real values fully quantify the relation between $\overleftrightarrow{C}'$ and $\overleftrightarrow{C}$ in Eq. (S4.12): 4 complex values for $\boldsymbol{T}$ evaluated at each point. Similarly, 16 real values are required to quantify the cross-scattering between a pair of generalized Stokes parameters vectors, and both formalisms are equally powerful. The conceptual difference between the two can be understood as: The values that relate the generalized Stokes parameters to each other quantify the change in statistics that the entire ensemble undergoes, while the Jones matrix quantifies the action upon a single realization in the ensemble. Using Eq. (S4.6), an analytic relation between these sets of values is easy to establish.

Our preference to formulate our polarization-aware light-matter interaction theory (Theorem S4.1) using the generalized Stokes parameters stems from the very same fact that we have stressed in the paper: it is the statistical properties of the wave ensemble that dictate its observable properties. This makes the generalized Stokes parameters more appealing. Anyhow, the manner in which we arrange these 16 quantities is of little consequence, it is *computing these 16 quantities that is the difficult endevour.* In general, computing one of these values requires solving a scalar diffraction problem (viz. Theorem 3.1), which is the problem we tackle in the paper.

Related work. We briefly discuss a few work that consider such ABCD systems, with an emphasis on work that focus on the effects on the coherence of light. These work deal with simple optical elements, where the Jones matrix can be formulated with relative ease, and none discuss the more general problem of diffraction with more complicated scatters. Therefore, these work are at most tangentially related and we cite a select few.

Shirai and Wolf [2004] as well as follow-up work by Hanson et al. [2008] consider ABCD systems that are composed of a free-space propagator, random phase screens and apertures with Gaussian-shaped transmission. A general discussion on liquid-crystal spatial light modulators to control coherence and polarization is given by Ostrovsky et al. [2011], and Ma et al. [2015] study the changes on the degree-of-coherence and degree-of-polarization induced on refraction through a rough-surfaced depolarizer.

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