Supplementary Material for:

Toward a Perfect Lens: Automated Design of GRIN Double-Freeform Systems for Broadband Aberration and Chromaticity Correction

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S1 Theoretical Principles and Physical Mechanisms

Traditional optical design relies heavily on local numerical ray tracing rooted in Fermat's principle, an approach inherently constrained from globally decoupling the independent contributions of respective surfaces. To actualize a non-iterative global inverse design, this paper embeds the system into an extended phase space, employing Lie algebra tools to map complex physical light paths into cascades of algebraic operators.

S1.1 Extended Phase Space and Lie Algebraic Modeling Incorporating Dispersion

In geometrical optics, ray evolution in phase space behaves according to Hamiltonian canonical equations. Integrating the dispersive characteristics of broad-band light sources into a comprehensive analytical domain necessitates establishing an extended phase space $\mathcal{P}_{\text{ext}} = T^*\mathbb{R}^2 \times \mathbb{R}^+ \times \mathbb{R}$,[1] which encompasses wavelength λ and its conjugate phase. On this manifold, the refractive index adopts a continuous functional form over spatial coordinates and wavelength: $n(\boldsymbol{q}, z, \lambda)$.

According to the Dragt-Finn factorization theorem,[2,3] any lossless optical mapping can be uniquely factorized into an infinite cascade of Lie transformations generated by homogeneous polynomials. Within the paradigm of the GRIN dual-freeform lens, the overarching transmission

mapping $\mathcal{M}_{\text{total}}$ from the object space to the image space is rigorously decomposable into the composition of three segregated physical procedures: refraction at the front freeform surface (operator $\mathcal{S}_1$), continuous Hamiltonian evolution through the interior GRIN medium (operator $\mathcal{D}_{\text{GRIN}}$), and refraction at the rear freeform surface (operator $\mathcal{S}_2$).

Utilizing the Baker-Campbell-Hausdorff (BCH) formula, these sequenced procedures can be consolidated into a unitary Lie transformation containing a total generator set $\{m_k(\lambda)\}_{k=2}^{\infty}$:

$$\mathcal{M}_{\text{total}}(\lambda) = \mathcal{S}_2 \circ \mathcal{D}_{\text{GRIN}} \circ \mathcal{S}_1 = \prod_{k=2}^{\infty} \exp(\{m_k(\lambda), \cdot\}) \tag{S1}$$

where $m_k(\lambda)$ embodies the overall system distribution of k-th order geometric and chromatic aberrations. Imposing the stringent physical prerequisites for perfect broadband imaging dictates that at the reference wavelength λ_0, all nonlinear geometrical aberrations are annihilated (i.e., $m_k^{(0)} = 0$), and simultaneously, the mapping manifests translational invariance with respect to wavelength (zeroing out primary dispersion: $m_k^{(1)} = \partial m_k/\partial\lambda|_{\lambda=\lambda_0} = 0$).

S1.2 Global Chromatic Compensation Mechanism Driven by Spatial Dispersion Gradients

The algebraic root describing why uniform single-media lenses fail to achieve achromatization lies in the fact that conventional materials present a dispersion rate ($\partial n/\partial\lambda$) that is overwhelmingly positive and spatially invariant. This induces a strictly unidirectional accumulation of overall dispersion generators, barring any self-cancellation.

The pivotal breakthrough reported herein involves unraveling the unique physical implications instantiated by the interplay between GRIN media and freeform geometries. By imposing the BCH expansion onto the total second-order generator (dominating primary longitudinal and transverse chromatic aberrations) and differentiating with respect to wavelength, the global chromatic compensation equation arises:

$$m_2^{(1)} = \frac{\partial s_2^{(1)}}{\partial\lambda} + \frac{\partial d_2}{\partial\lambda} + \frac{\partial s_2^{(2)}}{\partial\lambda} + \frac{1}{2}\left\{\frac{\partial s_2^{(1)}}{\partial\lambda}, d_2\right\} + \frac{1}{2}\left\{s_2^{(1)}, \frac{\partial d_2}{\partial\lambda}\right\} + \cdots = 0 \tag{S2}$$

Equation (S2) deeply encapsulates the geometric substance underlying broadband achromatization: separate from the fundamental dispersion supplied by the respective physical surfaces

(terms one and three), there are crucial nonlinear cross-coupling influences fabricated by Lie brackets.

Within this scaffolding, allocating a **spatial dispersion gradient** inside the GRIN medium (i.e., a refractive index profile mutating with wavelength, $\partial^2 n/\partial \boldsymbol{q} \partial \lambda \neq \mathbf{0}$) implies that light beams permeating different strata undergo not only diverging optical path variations but correspondingly fierce variations in encountered dispersion rates. By strictly interpreting the medium transmission generator $\partial d_2/\partial \lambda$ through Equation (S2), this spatial dispersion gradient proves capable of analytically inciting intensely powerful "anomalous negative chromatic aberration" properties (corresponding to the Lie bracket cross-terms). In phase space, this negative chromaticity perfectly offsets the uniformly positive chromatic aberrations sourced from the forefront and rear interfaces. The elimination of higher-order spherochromatism and chromatic coma obeys analogous deductive mechanisms.

S1.3 High-Dimensional Recursive Order-Reduction Algorithm for Nonlinear Systems

Through the designated mechanisms, highly intractable broadband system optimization demands map uniformly into a mathematically determinate system of partial differential equations: $m_k^{(0)} = 0$ and $m_k^{(1)} = 0$. Benefiting from the polynomial degree-lowering principle governing Lie Poisson brackets ($\{f_n, g_m\} \in \mathcal{P}_{n+m-2}$), this high-dimensional nonlinear coupling equation inherently expresses an elegant recursive resolvability. We propose a "bottom-up" stepwise dimensional reduction inversion algorithm:

1. **First-order solving (base geometries and primary achromatization, $k = 2$):** Direct resolution of linear polynomial identities analytically defines the interface base curvature tensors juxtaposed alongside the center index and radial dispersion gradients of the internal GRIN medium.

2. **Second-order solving (asymmetric topologies and distortion compensation, $k = 3$):** Substituting second-order variables into the third-order generators forces superior cross-terms to collapse into easily defined linear combinations, straightaway exposing the third-order surface topology variables corresponding to freeform geometries.

3. **High-order solving (spherical aberration, astigmatism, and high-order chromaticity, $k \geq 4$):** Advancing step-wise up the cascade logic, integrations traversing internal thickness along with higher-order medium tensors expose the ultimate freeform parameters guaranteeing the nullification of high-order discrepancies.

By circumventing traditional computation constraints associated with monumental brute ray-tracing repetitions, this algorithmic substitution structurally assures theoretical absolute global solution convergence.

S2 Extended Phase Space and Symplectic Geometry Theoretical Framework

To rigorously investigate aberration and chromatic features inside GRIN dual-freeform singlets, a comprehensive analytic model addressing spatial distortion and wavelength variances simultaneously is requisite. This section leverages Dragt-Finn factorization inside symplectic geometries to form the extended optical phase space containing wavelength distributions, transforming physical aims into strictly formalized algebraic equivalencies.

S2.1 Optical Hamiltonian Flow and Lie Transformation Factorization

In geometrical optics, coordinates characterizing a ray within the phase space $T^*\mathbb{R}^2$ encompass spatial transverse coordinates $\boldsymbol{q} = (q_1, q_2)^T$ combined with transverse optical momenta (direction cosines) $\boldsymbol{p} = (p_1, p_2)^T$, shaping a four-dimensional vector $\boldsymbol{w} = (\boldsymbol{q}, \boldsymbol{p})^T$. Ray propagation evolving along the primary optical axis z aligns squarely with Hamiltonian system dynamics[4] dictated by:

$$H_{\text{opt}}(\boldsymbol{q}, \boldsymbol{p}, z) = -\sqrt{n^2(\boldsymbol{q}, z) - |\boldsymbol{p}|^2} \tag{S3}$$

where $n(\boldsymbol{q}, z)$ specifies the spatial index distribution positioned at $(\boldsymbol{q}, z)$.

Propagation laws heed canonical Hamiltonian dictates $\mathrm{d}\boldsymbol{w}/\mathrm{d}z = J\nabla_{\boldsymbol{w}} H_{\text{opt}}$, engaging the standard symplectic matrix J. Maintaining symplectic preservation across canonical space directly relates back to lossless optical environments conforming to the geometric invariants mapped as $\omega_0 = \mathrm{d}\boldsymbol{q} \wedge \mathrm{d}\boldsymbol{p}$, and subsequently mirroring the foundational conservation inherent in optical etendue. As such, any fully lossless operation is interpretable simply as an analytic

symplectic mapping $\mathcal{M} : \mathbb{R}^4 \to \mathbb{R}^4$.

Per the Dragt-Finn decomposition theorem,[2] every analytical symplectic transform honoring $\mathcal{M}(\mathbf{0}) = \mathbf{0}$ yields seamlessly into sequential concatenations via Lie transforms governed by homogeneous polynomials $f_m \in \mathcal{P}_m$:

$$\mathcal{M} = \exp(\{f_2, \cdot\}) \circ \exp(\{f_3, \cdot\}) \circ \exp(\{f_4, \cdot\}) \circ \cdots = \prod_{m=2}^{\infty} \exp(\{f_m, \cdot\}) \tag{S4}$$

where $\{\cdot, \cdot\}$ refers to the Poisson bracket, and $\exp(\{f_m, \cdot\})$ acts as the defining operation within the exponentiated Lie mapping series.

S2.2 Constructing Wavelength-Inclusive Extended Phase Spaces

Standard Dragt-Finn methodologies apply to purely isolated monochromatic regimes. Unlocking chromatic capabilities requests stretching parameters bounding $T^*\mathbb{R}^2$ outwardly, encompassing wavelength variables $\lambda \in \mathbb{R}^+$ alongside its standardized optical-phase conjugate mapping metric $\phi \in \mathbb{R}$.

Defining optics into an **Extended phase space** establishes a distinct six-dimensional framework $\mathcal{P}_{\text{ext}} = T^*\mathbb{R}^2 \times \mathbb{R}^+ \times \mathbb{R}$, structured upon vectors $(\boldsymbol{q}, \boldsymbol{p}, \lambda, \phi)$. Integrating an expanded symplectic form:

$$\Omega = \omega_0 + \mathrm{d}\lambda \wedge \mathrm{d}\phi = \sum_{i=1}^{2} \mathrm{d}q_i \wedge \mathrm{d}p_i + \mathrm{d}\lambda \wedge \mathrm{d}\phi \tag{S5}$$

Due to factors ensuring $\mathrm{d}\Omega = 0$ alongside non-degeneracy protocols, $(\mathcal{P}_{\text{ext}}, \Omega)$ crafts flawless symplectic continuity. Wideband dispersion constraints denote index variables analytically bound as functions over sequential metrics $n = n(\boldsymbol{q}, z, \lambda)$. Therefore, the extended Hamiltonian registers $\mathcal{H}_{\text{ext}} = -\sqrt{n^2(\boldsymbol{q}, z, \lambda) - |\boldsymbol{p}|^2}$.

As analytic optical mappings $\mathcal{M}(\lambda)$ align fundamentally with variations against λ, an evaluation executed at precisely the median designated reference mark λ_0 translates specific structural values $f_m(\boldsymbol{q}, \boldsymbol{p}, \lambda)$ seamlessly into a cohesive Taylor series tracking offset ranges $(\lambda - \lambda_0)$:

$$f_m(\lambda) = f_m^{(0)} + (\lambda - \lambda_0) f_m^{(1)} + \frac{1}{2}(\lambda - \lambda_0)^2 f_m^{(2)} + \cdots \tag{S6}$$

Here, the derivative matrix $f_m^{(k)} = \frac{1}{k!} \frac{\partial^k f_m}{\partial \lambda^k}\big|_{\lambda=\lambda_0}$ is designated explicitly as the respective system's **k-th order chromatic aberration generator**.

S2.3 Algebraic Reconstruction of Broadband High-Order Aberration Cancellation

Deconstructing overarching mapping parameters guiding light arrays sequentially traversing diverse geometric layouts necessitates applying mathematical Baker-Campbell-Hausdorff (BCH) protocols. Any extensively convoluted operation collapses definitively targeting singular exponential transform groupings bearing cumulative summation values mapping overall systems tracking unified sets inside $\{m_k(\lambda)\}_{k=2}^{\infty}$:

$$\mathcal{M}_{\text{total}}(\lambda) = \prod_{k=2}^{\infty} \exp(\{m_k(\lambda), \cdot\}) \tag{S7}$$

Perfection bounds demand two unique partial-derivative criteria strictly maintained concurrently:

Constraint One: Overall Geometric Uniformity (Monochromatic Resolution) Eliminating sweeping distortion requires the strict vanishing of any nonlinear tracking metric evaluated precisely near established median bounds λ_0:

$$m_k^{(0)}(\boldsymbol{q}, \boldsymbol{p}) = 0, \quad \forall k \geq 3 \tag{S8}$$

Constraint Two: Uncompromising Chromatic Vector Control (Broadband Elimination) Evaluating overarching geometric linear progression constraints insists operational frameworks must uphold functional parity immune to wavelength fluctuations (nullification marking specific primary deviations):

$$m_k^{(1)}(\boldsymbol{q}, \boldsymbol{p}) = \left. \frac{\partial m_k}{\partial \lambda} \right|_{\lambda=\lambda_0} = 0, \quad \forall k \geq 2 \tag{S9}$$

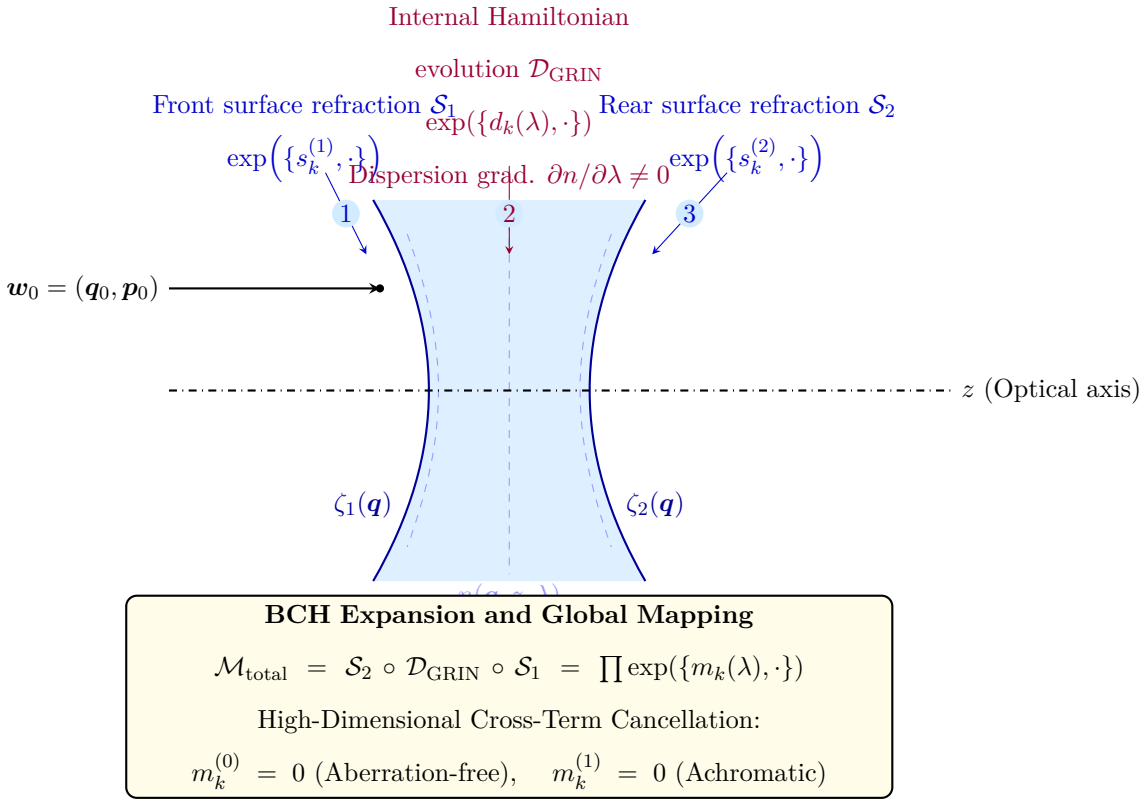


Figure S1: Diagram of Hamiltonian flow evolution and Lie transformation cascade factorization for a gradient-index dual-freeform lens in extended phase space.

S3 Lie Algebraic Modeling of Freeform Surfaces and GRIN Media

S3.1 Root Transformation of Refraction at Freeform Interfaces

Assume the front and rear freeform surfaces of the lens are described by profile functions $z = \zeta_1(\boldsymbol{q})$ and $z = \zeta_2(\boldsymbol{q})$. In the local coordinate system near the vertex, the interface is expanded as a Taylor series:

$$\zeta(\boldsymbol{q}) = \frac{1}{2}\boldsymbol{q}^T\boldsymbol{C}\boldsymbol{q} + \frac{1}{6}S_{ijk}q_iq_jq_k + \frac{1}{24}T_{ijkl}q_iq_jq_kq_l + \cdots \tag{S10}$$

where $\boldsymbol{C}$ is the second-order curvature matrix, and S_{ijk} and T_{ijkl} control the third- and fourth-order asymmetric freeform topologies.

For the front surface $\zeta_1(\boldsymbol{q})$ refracting from air ($n_0 = 1$) into the dispersive medium $n(\lambda)$, its

first three generators $s_k^{(1)}(\boldsymbol{q}, \boldsymbol{p}, \lambda)$ are:

$$s_2^{(1)} = -\frac{1}{2}(n(\lambda) - 1)\boldsymbol{q}^T \boldsymbol{C}_1 \boldsymbol{q} \tag{S11}$$

$$s_3^{(1)} = -\frac{1}{6}(n(\lambda) - 1) S_{ijk}^{(1)} q_i q_j q_k \tag{S12}$$

$$s_4^{(1)} = -\frac{1}{24}(n(\lambda) - 1) T_{ijkl}^{(1)} q_i q_j q_k q_l + \frac{n(\lambda) - 1}{4n(\lambda)} |\boldsymbol{p}|^2 (\boldsymbol{q}^T \boldsymbol{C}_1 \boldsymbol{q}) - \frac{(n(\lambda) - 1)^2}{8n(\lambda)} (\boldsymbol{q}^T \boldsymbol{C}_1 \boldsymbol{q})^2 \tag{S13}$$

Crucially, the refraction generator s_k explicitly depends on wavelength λ. Differentiating with respect to λ uncovers the intrinsic chromatic tensor of the surface.

S3.2 Symplectic Transformation of Internal GRIN Propagation

Inside the lens, ray trajectories are determined by the symplectic flow driven by the extended Hamiltonian $\mathcal{H}_{\text{ext}}$. To maximize the degrees of freedom for aberration compensation, the refractive index field is expanded into a mixed polynomial incorporating spatial and dispersion gradients:

$$n^2(\boldsymbol{q}, z, \lambda) = N_0^2(z, \lambda) - N_1(z, \lambda)|\boldsymbol{q}|^2 - \sum_{i+j=3} N_{ij}(z, \lambda) q_1^i q_2^j - \sum_{i+j=4} M_{ij}(z, \lambda) q_1^i q_2^j + \cdots \tag{S14}$$

Correspondingly expanding $\mathcal{H}_{\text{ext}} = H_2 + H_3 + H_4 + \cdots$:

$$H_2 = -N_0(z, \lambda) + \frac{|\boldsymbol{p}|^2}{2N_0(z, \lambda)} + \frac{N_1(z, \lambda)|\boldsymbol{q}|^2}{2N_0(z, \lambda)} \tag{S15}$$

$$H_3 = \frac{\sum N_{ij} q_1^i q_2^j}{2N_0(z, \lambda)} \tag{S16}$$

$$H_4 = \frac{\sum M_{ij} q_1^i q_2^j}{2N_0(z, \lambda)} + \frac{|\boldsymbol{p}|^4}{8N_0^3(z, \lambda)} + \frac{N_1(z, \lambda)|\boldsymbol{p}|^2|\boldsymbol{q}|^2}{4N_0^3(z, \lambda)} + \frac{N_1^2(z, \lambda)|\boldsymbol{q}|^4}{8N_0^3(z, \lambda)} \tag{S17}$$

The internal propagation operator $\mathcal{D}_{\text{GRIN}}$ decomposes into $\exp(\{d_2, \cdot\}) \circ \exp(\{d_3, \cdot\}) \circ \exp(\{d_4, \cdot\}) \circ \cdots$. The generator d_k is obtained by integrating the respective Hamiltonian orders:

$$d_2(\lambda) = -\int_{z_1}^{z_2} H_2(\boldsymbol{q}(z), \boldsymbol{p}(z), z, \lambda) \mathrm{d}z \tag{S18}$$

$$d_m(\lambda) = -\int_{z_1}^{z_2} \tilde{H}_m(\boldsymbol{q}(z), \boldsymbol{p}(z), z, \lambda) \mathrm{d}z, \quad \forall m \geq 3 \tag{S19}$$

S4 Conditions for Stepwise Cancellation of Geometric and Chromatic Aberrations

S4.1 BCH Concatenation of the Total Symplectic Mapping

Applying the BCH formula, the exponential operators combine. The Poisson bracket enforces degree-lowering: $\{f, g\} \in \mathcal{P}_{n+m-2}$ for $f \in \mathcal{P}_n$ and $g \in \mathcal{P}_m$. This groups the total generator m_k analytically:

$$m_2 = s_2^{(1)} + d_2 + s_2^{(2)} + \frac{1}{2}\{s_2^{(1)}, d_2\} + \frac{1}{2}\{d_2, s_2^{(2)}\} + \frac{1}{2}\{s_2^{(1)}, s_2^{(2)}\} + \cdots \tag{S20}$$

$$m_3 = s_3^{(1)} + d_3 + s_3^{(2)} + \frac{1}{2}\{s_2^{(1)}, d_3\} + \frac{1}{2}\{s_3^{(1)}, d_2\} + \cdots \tag{S21}$$

$$m_4 = s_4^{(1)} + d_4 + s_4^{(2)} + \frac{1}{2}\{s_2^{(1)}, d_4\} + \frac{1}{2}\{s_4^{(1)}, d_2\} + \frac{1}{2}\{s_3^{(1)}, d_3\} + \cdots \tag{S22}$$

These expansions prove that total aberrations transcend mere linear summations of individual element aberrations.

S4.2 Elimination Theory for Monochromatic Geometric Aberration

The criterion for resolving monochromatic aberrations dictates $m_k^{(0)} = 0$ ($\forall k \geq 3$). Taking third-order geometric aberration ($k = 4$) as an example, nullifying Equation (S22) yields:

$$s_4^{(1)} + s_4^{(2)} + d_4 + \mathcal{X}_4(s_2, s_3, d_2, d_3) = 0 \tag{S23}$$

where $\mathcal{X}_4$ aggregates all high-order cross-terms. By introducing high-order spatial gradient polynomials inside the internal index profile M_{ij}, the algebraic structure theoretically secures an exact global resolution ensuring $m_k^{(0)} = 0$.

S4.3 Gradient Dispersion Compensation for Broadband Chromaticity

For broadband chromaticity cancellation, mapping evolution insists on wavelength invariance ($m_k^{(1)} = 0$). By differentiating Equation (S20) with respect to wavelength, the chromatic com-

pensation equation presents:

$$m_2^{(1)} = \frac{\partial s_2^{(1)}}{\partial \lambda} + \frac{\partial d_2}{\partial \lambda} + \frac{\partial s_2^{(2)}}{\partial \lambda} + \frac{1}{2}\left\{\frac{\partial s_2^{(1)}}{\partial \lambda}, d_2\right\} + \frac{1}{2}\left\{s_2^{(1)}, \frac{\partial d_2}{\partial \lambda}\right\} + \cdots = 0 \tag{S24}$$

In the GRIN medium, specifying a **spatial dispersion gradient** ($\partial N_1/\partial\lambda \neq 0$) mathematically infuses formidable anomalous negative chromatic potential directly through the derivation of $\partial d_2/\partial\lambda$. Modulating the gradient dispersion tensor strategically provokes these negative terms to absolutely counteract the ubiquitous uniform positive dispersion intrinsic to boundary refractions via geometrical phase-space cross-term twisting.

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