Momentum Analysis for Metasurfaces

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Utilizing discrete phase distribution to fit continuous phase distribution has been a primary routine for designing metasurfaces. In the existing method, the validation of the discrete designs is guaranteed only by using the sub-wavelength condition of unit cells, which is insufficient, especially for arbitrary phase distribution. Herein, we proposed an analytical method to design metasurfaces via estimating the width of the source in a unit cell. Also, by calculating field patterns in both real- and momentum-space, we provided four guidelines to direct future applications of metasurfaces, such as an arbitrary multi-foci lens with the same strength of each focus, a convex-concave double lens, and a lens with a large numerical aperture that can precisely prevent undesired diffraction orders. Besides metalens, this methodology can provide a wide platform for designing tailored and multifunctional metasurfaces in future, especially large-area ones in practical applications.

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I. INTRODUCTION

Artificially engineered metasurfaces, comprising a dense arrangement of sub-wavelength resonators, are efficient and facilely fabricated substitution of bulk metamaterials [1–5]. By introducing an abrupt phase shift to the incident wavefront, metasurfaces modify the scattered wavefront in deep sub-wavelength scale, such as anomalous refraction [6, 7], metalenses [8–10], holographic plates [11–13], coding metasurfaces [14], wave plates [15], and asymmetric transmission [16–18]. Other novel applications including spin Hall Effect [19], topological transitions [20, 21], and nonlinear responses [22, 23] are also proposed with specific design of metasurfaces. It has been demonstrated that the generalized refraction is equivalent to blazed diffraction gratings [6, 24]. However, the existing quantitative diffracting theories mainly handle either a linearly distributed phase profile or holography, which is highly insufficient compared with the modulation depth of the metasurfaces. In addition, these theories always treat the discontinuous phase distribution as quasi-continuous, which is valid for most of the existing metasurfaces. However, when the phase of each unit cell varies abruptly, or the size of the unit cell is close to or even larger than the wavelength in nonlinear metasurfaces [22], the hypothesis of quasi-continuous is no longer validated.

Recently, metasurface holography enabling arbitrary wavefront reconstruction and optical communication has attracted considerable research interests in the scientific community [25, 26]. Unlike the traditional holograms, which is generated by interference of a reference beam with the scattered beam from a real object, the metasurface hologram is generated by numerically computing the phase information at the hologram interface using the computer-generated holography (CGH) method [27]. With delicately controlled geometry of the antennas, the desired phase profile can be achieved to accomplish three-dimensional holography [28], surface plasmon holography [29], multiwavelength achromatic holography [30], and nonlinear holography [31]. Using reflectivetype plasmonic metasurfaces [32] and dielectric Huygens metasurface [33], high-efficiency holograms can also be realized. It is known that holography is based on Fourier analysis to achieve information storage or image reconstruction. Fourier analysis is indeed a more fundamental theory, that can describe the scattered diffraction field for most of the metasurfaces besides holographic metasurfaces. However, the corresponding analyzing method has not been applied to an arbitrary metasurface, such as metalens.

Moreover, the reflection’s law, regular or generalized Snell’s law, and the grating equation are all derived from a single principle: conservation of momentum along the surface of the device (Demonstrated in Appendix A). Momentum, which is wave vector in electrodynamics, as well as energy are always dominant quantities. Herein, we provide a general guide to evaluate the diffracting field emitted from an arbitrarily arranged metasurface, with tailored functionalities but without considering the specific nanostructures or material details. First, we proposed a localized hypothesis of the unit cells composing metasurfaces. The sizes of source in the unit cells are in consideration compared with other works, in which the unit cells are just characterized by a point source with an effective dipole moment [34] or multipolar components [35]. Second, we employed the Fourier analysis to derive a generic wavefront in \( k \)-space. We provided four guidelines for designing metasurfaces based on this momentum analyzing method, the most important one of which is the stable condition that fulfills the conditions to mimic continuous phase distribution using a discontinuous phase profile. Taking metalens as an example, we
realized an arbitrary periodic-foci lens, a convex-concave double lens, and a large numerical aperture (NA) lens preventing undesired diffracting orders via the derived formulas. Our results provide a powerful tool to design the advanced functional and tunable metadevices, especially large-area ones in practical applications.

II. MODELING APPROACH

The strength and phase of output light are two main parameters that facilitate the design of tailorable metasurfaces. When any two adjacent unit cells are weakly-coupling (UCWC), these two parameters can characterize an independent unit cell regardless of the radiation type of the nanostructure [6–18, 28–33, 36]. Based on this designing strategy, the responding function of a unit cell can be mathematically defined as a rectangular function \( t(x) = |t_i| \text{rect}(x/T_{MS}) e^{-i\phi_i} \), where \( |t_i| \) is the responding strength (reflection or transmission) and \( \phi_i \) is the phase delay of the unit cell. The factor \( \text{rect}(x/T_{MS}) \) is the estimation of the locality for the unit cell, where \( T_{MS} \) describes an equivalent size that the nanostructure can govern, as illustrated in Fig. 1(a). When the parameter of width \( T_{MS} \) is small enough comparing with the resonant wavelength, the radiating nanostructure can be treated as a point source. Generally, the actual value of \( T_{MS} \) should be decided via the geometry and materials of the nanostructures in a unit cell, and can be simply estimated by the size of the nanostructure. In Appendix B, we compared our theory with the experimental results in Ref. [6] and simulated results in Ref. [37], where the \( T_{MS} \) is set as the size of the nanostructures. The far field diffraction pattern is the Fourier transform of the responding function based on the principle of superposition [38]:

\[
F(k) = \frac{|t_i|}{\pi} \sin(kT_{MS}/2) e^{-i\phi_i}.
\]

Equations (4) and (5) express the far field diffraction patterns for all UCWC metasurfaces. Specifically, the diffracting field of a metasurface \( M_1 \) with \( N \) unit cells is

\[
F(k) = \sum_{i=1}^N \frac{|t_i|}{\pi} \sin(kT_{MS}/2) e^{-i(\phi_i + kx_i)}.
\]

For simplicity, \( |t_i| \equiv 1 \) and \( T_{MS} \equiv T_{MS} \ll \lambda \) are assumed. Then,

\[
F(k) \propto F_1(k) \equiv \sum_{i=1}^N e^{-i(\phi_i + kx_i)}.
\]
Consider another metasurface $M_2$ with a diffracting field of

$$\mathcal{F}_2(k) \equiv \sum_{i=1}^{N/2} e^{-i(\phi_{2i} + kx_{2i})}. \quad (7)$$

$M_2$ is obviously composed of all the even unit cells in $M_1$. If the diffracting field of $M_2$ converges, the field should be analogous to the diffracting field of $M_1$, which implies that

$$\mathcal{F}_2(k) \propto \mathcal{F}_1(k). \quad (8)$$

On the other hand, $\mathcal{F}_1(k)$ and $\mathcal{F}_2(k)$ are related mathematically by

$$\sum_{i=1}^{N} e^{-i(\phi_i + kx_i)} = \sum_{i=1}^{N/2} \left(1 + e^{i\Delta\phi_{2i}} e^{i(k\Delta x_{2i})}e^{-i(\phi_{2i} + kx_{2i})} \right), \quad (9)$$

where $\Delta\phi_{2i} = \phi_{2i} - \phi_{2i-1}$, $\Delta x_{2i} = x_{2i} - x_{2i-1}$.

Comparing Eqs. (6)–(9), the Eq. (8) can be satisfied only when the coefficients of $1 + e^{i\Delta\phi_{2i}} e^{i(k\Delta x_{2i})}$ in Eq. (9) equal to a constant for every $i$ and $k$. Thus, we attain the conditions for discrete phase distribution to mimic a continuous phase distribution:

$$k\Delta x_{2i} \ll 2\pi, \quad (10)$$

$$\Delta\phi_{2i} \simeq C. \quad (11)$$

Generally, the subscript $2i$ can be replaced by $i$. The Eq. (10) is exactly the sub-wavelength condition, which can be simply written as $\Delta x \ll \lambda$. When the phase of each unit cell varies rapidly, Eq. (11) will be nullified, and the sub-wavelength condition will not guarantee validation of mimicking a continuous phase distribution. Specifically, $\Delta\phi_i \simeq 0$ means phase of the unit cell varies slowly. Equation (11) is called as stable condition in this study.

For an arbitrary phase distribution, the following four issues are important:

1. One-to-one correspondence. Each unit cell produces a plane wave in $k$-space, and each harmonic component in $k$-space corresponds to a unit cell.

2. Randomness. All the wavefront should be considered since $n$ is any integer in Eq. (3).

3. Stable condition Eq. (11). In contrary to the general case, the condition of sub-wavelength is not sufficient to mimic a continuous phase distribution, and the stable condition should also be accomplished.

4. Evanescent waves. Although $|k| \leq k_0$ (wavevector in free space) should be satisfied for all propagating waves, solutions to Eq. (3) with large values of $n$ must exist due to the principle of the phase uncertainty.

![FIG. 2: (color online) Multi-focus metalens with a lattice size of 700 nm, focal length of 20 μm operating at a wavelength of 1 μm. (a) Parabolic and its normalized phase distribution of discrete unit cells along x-axis. The red and blue areas indicate different regions of the metalens that serve as independent foci. (b) Phase difference of the adjacent unit cells with a lattice size of 700 nm (blue dotted line) and 350 nm (green dotted line). (c) Amplitude distribution of a two-focus metalens. (d) Amplitude distribution of a five-focus metalens.](image)

### III. APPLICATIONS IN METALENS

#### A. ARBITRARY MULTI-FOCI METALENS

The necessity of stable condition can be interpreted through a metalens. It is well known that a hyperbolic phase profile equals to a parabolic phase distribution under the paraxial approximation, which is commonly used to simplify the design of a metalens [39]. However, if the phase profile is defined as $\varphi(x) = k_0x^2/2f$, a two-dimensional multi-focus metalens can be achieved when $x$ covers a large range, as shown in Fig. 2. The designed metalens has a unit size of 700 nm and focal length of 20 μm operating at a wavelength of 1 μm. Interestingly, the original phase profile and the normalized phase profile are both aperiodic [Fig. 2(a)]; however, the focusing profile is periodic. We designed this multifocus lens to demonstrate the stable condition, which is different with the theory in Ref. [40]. Evidently this metalens breaks the stable condition $\Delta\phi_i \simeq C$. As illustrated in Fig. 2(b), the phase difference between two adjacent unit cells varies periodically from $-\pi$ to $\pi$, which cannot be considered close to a constant. To theoretically derive this unique phenomenon, let us first consider the phase difference between two adjacent unit cells. Assuming the size of the unit cells is fixed as $\Lambda$, the phase difference is $\Delta\varphi(n\Lambda) = \varphi((m+1)\Lambda) - \varphi(m\Lambda) = k_0\Lambda^2(1+2m)/2f$, where $m$ is an integer representing the $m$th unit cell. Thus, the localized wave vector is $k_m = -\Delta\varphi/\Lambda = -k_0(1+2m)/2f$. If the focus of the system is periodic, the localized wave
vector should also be periodic. Considering the randomness of the phase, we can obtain the following formula:

$$k_{m+a} = k_m - \frac{2n\pi}{\Lambda},$$

where \(a\) is also an integer representing the number of unit cells for each period. Equation (12) can be precisely solved:

$$a\Lambda = \frac{2n\pi f}{k_0\Lambda}. \quad (13)$$

Thus, when \(n = 1\) the minimum period of the foci can be calculated as 28.6 \(\mu m\) from Eq. (13), which is in agreement with the simulated results in Fig. 2(c). Another interesting phenomenon is that although the size of the unit cell is less than the wavelength, the diffracting field is much different from that of a continuous phase distribution. According to Eq. (13), even when \(\Lambda = \frac{\lambda}{10}\), the period of the foci is \(10f\), which is still not converged. Furthermore, Eq. (13) can be reformed as:

$$\Lambda \left( \frac{a\Lambda}{f} \right) = n\lambda. \quad (14)$$

Compared this equation with the grating equation \(A\sin \theta = n\lambda\), the designed multi-foci metalens is indeed a beam splitter just like a grating. However, for the gratings, \(|\sin \theta| \leq 1\) is maintained; whereas, for the metalens, \(a\Lambda/f\) can theoretically be arbitrarily designed. The numbers of foci are linearly proportional to the size of the metalens according to Eq. (13). A five-foci metalens is shown in Fig. 2(d), with the same foci distance of 28.6 \(\mu m\). It should be noticed that the amplitudes of the foci are equal due to the periodicity of the localized wave vector originating from the phase gradient of the metalens. The metalens can serve as a generalized grating with the same strength for all the diffracting orders.

**B. CONVEX-CONCAVE DOUBLE LENS**

We also used the proposed theory to design a convex-concave double lens. The unit cells of the metasurface are located at a hyperbolic phase distribution \(\varphi(x) = k_0(\sqrt{x^2 + f^2} - f) = n\pi \quad (n \in \mathbb{N})\), as indicated using red dots in Fig. 3(a). It is obvious that these units can generate a focused wavefront [Fig. 3(c)]. However, due to the randomness of the phase, the phase profile can also be projected to another function \(\varphi(x) = -k_0(\sqrt{x^2 + f^2} - f) = -n\pi \quad (n \in \mathbb{N})\), which can simultaneously achieve a concave lens [Fig. 3(b)]. Similarly, if the blue doted phase profile in Fig. 3(a) is first designed, the red doted one will occur as well. The one-to-one mapping conjugate phase configuration indicates that this device can converge or diverge an incident photon with the same probability. As shown in Fig. 3(d), the amplitudes of real and virtual F are both 0.55 according to the simulation, which implies that convex and concave equally serve the functionality of the device. The transmitted field in the white solid box in Fig. 3(d) is totally mirror-symmetric to the conjugate zone, and this is a direct consequence of the one-to-one mapping conjugate phase configuration.

To further examine the exact diffraction patterns of

**FIG. 3:** (color online) Designed convex-concave double lens with focal length of 5 \(\mu m\) operating at a wavelength of 1 \(\mu m\). (a) Phase distribution along the \(x\)-axis (red dots) and its image phase distribution (blue dots). Locations of integral \(\pi\) are picked up to locate the unit cells of the lens. (b)-(c) Transmitted field profile of the diverged and focused wavefronts. (d) Strength distribution of the transmitted field (white solid box) and effective incident field (white dashed box). The real and virtual focus are both depicted.

**FIG. 4:** (color online) Calculated \(J\)-parameters for (a) focusing metalens, (b) diverging metalens, (c) left side of the focusing metalens, (d) left side of the diverging metalens, (e) left side of the convex-concave double lens with 20 unit cells, (f) left side of the convex-concave double lens with 100 unit cells. Insets: schematics of all the above-mentioned devices. Metalenses in (a)-(d) are designed with a unit size of 500 nm and a focal length of 5 \(\mu m\) operating at wavelength of 1 \(\mu m\).
the output field, we calculated the $F$-parameters in Eq. (5) for the regular focusing metalens, the regular diverging metalens, and the convex-concave double lens, respectively. In Fig. 4, the horizontal ordinate of the graph is calculated through $\theta = \arcsin(k_f/k_0)$, characterizing the divergent angle of output light. The sharp peaks appearing in the lines are caused by the interference of the scattered field, which cannot be eliminated even after improving the calculating accuracy. Interestingly, one cannot recognize a convex and a concave lens from a far distance because a parallel incident light both diverges after passing the focus of the lens. As shown in Figs. 4(a) and 4(b), the $F$-parameters are the same for a convex and a concave metalens. To distinguish the two lenses, we only analyzed the left sides of the devices [Figs. 4(c) and 4(d)]. For a left-sided convex metalens (30 unit cells utilized), the transmitted light travels toward the right side ($\theta \geq 0$); whereas for a left-sided concave metalens, the transmitted light travels toward the left side ($\theta \leq 0$). In contrast, $F$-parameters for the left-sided convex-concave double lens are calculated in Fig. 4(e), which combine Fig. 4(c) with Fig. 4(d), demonstrating that it can simultaneously work as a convex lens and a concave lens. The minor differences between Figs. 4(e)–4(d) and Fig. 4(e) can be attributed to other orders of diffraction, which primarily exist when $|x|$ and $n$ is small. For example, with $x_1 = 0$ ($n = 0$) and $x_2 = -2.29 \mu m$ ($n = 1$), $-\nabla \varphi_0 = 0.22k_0$ can be obtained. Meanwhile, other phase gradients $-\nabla \varphi_n = -((\Delta \varphi + 2m\pi)/\Delta x) = \{-0.22k_0, 0.66k_0, -0.66k_0\}$ are permitted due to the randomness of phase. On the contrary, when $|x|$ or $n$ is large enough, $\Delta x$ can be less than a wavelength and $|2m\pi/\Delta x| > k_0$ is maintained for most of the integer $m$. In this situation, only the diffracting order of convex and concave lens can be satisfied and efficiency of each component can approach $\sim 0.5$. The numbers of unit cells are not important for evaluating the functionality of the devices though they can decide the peak position of the $F$-parameters. The divergent angle increases as the distance from the center of a lens increases. Thus, the $F$-parameters of an infinite lens should possess two large peaks around $90^\circ$ and $-90^\circ$. In Fig. 4(f), the $F$-parameters of the convex-concave double lens with 100 unit cells are calculated, which is totally in agreement with the intuitional expects. For all the calculation in Fig. 4, we assume $T_{MS}$ to be $300 \mu m$, around $\Lambda/3$. Results for different $T_{MS}$ values are also displayed in Fig. 9 in Appendix E.

C. LARGE NA METALENS

For the sub-wavelength hyperbolic metalens, the momentum analysis is also necessary especially when NA is large. Considering a phase profile $\varphi(m\Lambda) = k_0(\sqrt{(m\Lambda)^2 + f^2} - f)$, where $\Lambda$ is size of the unit cell. We can calculate the phase difference between two adjacent unit cells are not important for evaluating the function-

ia of the devices though they can decide the peak posi-

tion of the lenses. Meanwhile, other phase gradients $-\nabla \varphi_n = -((\Delta \varphi + 2m\pi)/\Delta x) = \{-0.22k_0, 0.66k_0, -0.66k_0\}$ are permitted due to the randomness of phase. On the contrary, when $|x|$ or $n$ is large enough, $\Delta x$ can be less than a wavelength and $|2m\pi/\Delta x| > k_0$ is maintained for most of the integer $m$. In this situation, only the diffracting order of convex and concave lens can be satisfied and efficiency of each component can approach $\sim 0.5$. The numbers of unit cells are not important for evaluating the functionality of the devices though they can decide the peak position of the $F$-parameters. The divergent angle increases as the distance from the center of a lens increases. Thus, the $F$-parameters of an infinite lens should possess two large peaks around $90^\circ$ and $-90^\circ$. In Fig. 4(f), the $F$-parameters of the convex-concave double lens with 100 unit cells are calculated, which is totally in agreement with the intuitional expects. For all the calculation in Fig. 4, we assume $T_{MS}$ to be $300 \mu m$, around $\Lambda/3$. Results for different $T_{MS}$ values are also displayed in Fig. 9 in Appendix E.

![Image](image_url)

**FIG. 5:** (color online) A hyperbolic metalens with a large NA computed as 0.97 (total size of the lens is $700 \mu m$). The focal length is $80 \mu m$, operating at a wavelength of $1 \mu m$. Size of the unit cells is set to be $\beta \Lambda$. (a) Normalized phase difference between two adjacent unit cells with $\beta = 0.7$ (red solid line) and $\beta = 0.4$ (blue solid line). The dashed lines are asymptotic ones for the corresponding phase differences, on which asymptotic values are marked. (b) Simulated focusing field with $\beta = 0.7$, and the white dashed circles indicate zones of high-order diffraction. (c) Simulated focusing field with $\beta = 0.4$ without high-order diffractions. Computed $F$-parameters for (d) $\beta = 0.7$ and (e) $\beta = 0.4$. Considering the sub-wavelength condition $0 < \beta < 1$ is often required, the solution of Eq. (16) is $\{n = 0, 0 \leq \beta < 1\}$, or $\{n = -1, 0.5 \leq \beta < 1\}$. When the NA of the metalens is large enough and $0.5 \leq \beta < 1$, the diffracting order of $-1$ will occur. As indicated by the white dashed circles in Fig. 5(b), an obvious diffraction occurs.
when \(|x| \geq 70\ \mu m\) in the case of \(\beta = 0.7\). In contrast, in the case of \(\beta = 0.4\), the high orders of diffraction are suppressed to near field evanescent components and only a focusing wavefront is permitted. An accurate method to evaluate diffraction is to calculate the \(F\)-parameters, as shown in Figs. 5(d) and 5(e). We can see that the \(F\)-parameter for \(\beta = 0.7\) has more peaks (diffracting wave vectors) around \(\pm 31.3^\circ\). However, the calculated \(F\)-parameter for \(\beta = 0.4\) is more smooth and only has two main peaks at around \(\pm 64.9^\circ\), which just overlap with the corresponding peaks for \(\beta = 0.7\).

IV. CONCLUSION

In conclusion, we have deduced an enhanced diffraction theory to evaluate the far field for an arbitrary UCWC metasurface, which is based on estimating the width of the source in a unit cell and performing Fourier transform of the unit cell’s responding function. We proposed four guidelines to design metasurfaces, especially when the sub-wavelength condition is no longer sufficient to fit a continuous phase distribution. According to the guidelines, the theory has been employed in applications such as: (I) an arbitrary multi-foci lens; (II) a convex-concave double lens; (III) a lens with a large NA preventing undesired diffraction orders. From the theoretical prediction as well as the computational results, the diffracting approach extended to arbitrary phase distributions has been demonstrated to be a powerful tool for guiding the design of multifunctional metasurfaces. Our approach provides a wide platform for designing tailored multifunctional, tunable, especially large-area metasurfaces in practical applications.

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APPENDIX A: CONSERVATION OF MOMENTUM FOR BASIC OPTICAL ELEMENTS

In quantum optics, momentum of a photon is linearly related to wave vector: \(p = \hbar k\). Thus, conservation of momentum also means conservation of wave vectors. The law of reflection states that \(\theta_r = \theta_i\), which can also be written as

\[ k_0 \sin \theta_r = k_0 \sin \theta_i \iff k_{||r} = k_{||i}. \]  

(A1)

The law of refraction states that \(n_i \sin \theta_i = n_t \sin \theta_t\), which also implies

\[ k_{||t} = k_{||i}. \]  

(A2)

The generalized Snell’s law states that \(n_t \sin \theta_t - n_i \sin \theta_i = (\lambda d\Phi)/(2\pi dx)\) [6], and it can be rewritten as

\[ k_{||t} - k_{||i} = k_A, \]  

(A3)

where \(k_A = d\Phi/dx\) is the phase gradient along the surface of the metasurface.

The equation of gratings is \(d(\sin \theta_i + \sin \theta_m) = m\lambda\), which can also be written as

\[ k_{||t} + k_{||d} = mk_d, \]  

(A4)

where \(k_d = 2\pi/d\) is the reciprocal lattice of the grating.

From Eqs. (A1)–(A4), we can see that the law of reflection, regular or generalized Snell’s law, and equation of gratings, all result from a single principle—conservation of wave vectors along the surface of the device—which motivated us to use \(F\)-parameters to characterize a flat optical elements–metasurface.

APPENDIX B: THEORY TEST

We utilized a simple metasurface grating to test our theory. In Fig. 6(a)–6(b), the metasurface possesses unity transmittance and same phase delay in each unit cell. The size of a unit cell is set as \(\Lambda = 2\lambda\) (\(\lambda\) is the incident wavelength). It is evident that the transmitted light can be scattered to higher orders of diffraction, \(\{0, \pm \frac{2\pi}{\Lambda}, \pm \frac{4\pi}{\Lambda}, \ldots\}\), corresponding to diffracting angles of \(\{0, \pm 30^\circ, \pm 90^\circ\}\) (higher orders become evanescent waves).

![FIG. 6: (color online) Computed \(F\)-parameters for the metasurface grating with an incident wavelength of 1 \(\mu m\) and unit cell of 2 \(\mu m\). (a) \(T^{MS} = 900\ \text{nm}\). Inset: schematic of the grating’s configuration. (b) \(T^{MS} = 300\ \text{nm}\). (c) Calculated first order anomalous refraction based on our theory to compare with Fig. 3(c) in Ref. [6]. In the calculation, \(T^{MS}\) is set as 1.3 \(\mu m\) (average size of all the V-shaped antennas taken from Ref. [6]). (d) Calculated scattered intensity based on our model to compare with Fig. 1(c) in Ref. [37]. In the calculation, \(T^{MS}\) is set as 1.12 \(\mu m\) (total size of the three waveguides).](image-url)
Figure 6(a)–6(b) depicts exactly the diffracting orders the metasurface can provide under the responding function (transmission or reflectance) \( t_i(x) = \text{rect}(x-x_i/T_{MS})e^{-i\phi} \). The blue lines correspond to the zeroth order diffraction, while the red lines indicate first order diffractions. It can be seen that the width of the source in a unit cell, \( T_{MS} \), mainly affects the relative strength of each diffracting order. In addition, with \( T_{MS} = 300 \) nm, the second order diffraction at nearly \( +90^\circ \) occurs although diffractions beyond \( 90^\circ \) evanesce and cannot be detected from far field. For a traditional grating, the responding function is exactly a rectangular function, while for an arbitrary metasurface, the factor \( \text{rect}(x/T_{MS}) \) is an equivalent estimation of a unit cell’s locality.

To test our theoretical model, we compared the experimental results in Ref. [6] with our calculated model. In our calculation, \( T_{MS} \) is set as \( 1.3 \mu m \) by averaging four basic Vshape antennas in Ref. [6]. The total size of the metasurface in the calculation is 230 \( \mu m \). The phase and intensity of each antenna are all taken from the reference. Specifically, besides the refraction angle, the height and width of 40 \( \mu m \), and thickness of 40 \( \mu m \). Orientation angle \( \theta \) is fixed at \( 90^\circ \) to get a PancharatnamBerry phase of \( 2n\pi \). (d) Intensity distribution of the convex-concave double lens.

The designed metasurfaces in the main text can be easily achieved. As an example, we used a two dimensional simulation with a dielectric metasurface to acquire a similar result with that of Fig. 2(c), as shown in Figs. 7(a)–7(b). The lattice size of the metasurface is 450 \( \mu m \) with a focal length of 20 \( \mu m \), operating at a wavelength of 1310 nm and the incident light is polarized along \( y \) direction. The height of the silicon structure is 1033 nm, and width \( w \) of the silicon is 95 nm, 120 nm, 135 nm, 160 nm, 205 nm, 250 nm, 300 nm, and 390 nm, respectively. The refraction index of silicon is set as 3.45. The simulated distance of two foci is \( D = 58.22 \mu m \), and the calculated distance according to Eq. 13 is 58.22 \( \mu m \) as well. We also used a plasmonic metasurface to achieve the convex-concave double lens. The positions of each gold antenna are depicted in Fig. 7(c), and the intensity distribution in Fig. 7(d) is consistent with that in Fig. 3(d).

**APPENDIX C: F-PARAMETERS FOR A TWO-DIMENSIONAL METASURFACE**

The responding function of the \( i \)th unit cell located at \( (x_i, y_i) \) can be written as

\[
T_i(x, y) = |t_i| \text{rect}(x-x_i/T_{MS})\text{rect}(y-y_i/T_{MS})e^{-i\phi_i}. \quad (C1)
\]

By performing a two-dimensional Fourier transform, the diffracting field in \( k \)-space is

\[
F_i(k_x, k_y) = \frac{|t_i|}{\pi} e^{-i(\phi_i + k_x x_i + k_y y_i)} \times \frac{\sin(k_x T_{MS}/2)}{k_x} \frac{\sin(k_y T_{MS}/2)}{k_y}.
\]

Thus, the total responding function and diffraction pattern should be

\[
T(r) = \sum_i |t_i| \prod_{v=x,y} \text{rect}(y-v/T_{MS}) e^{-i\phi_i}, \quad (C3)
\]

\[
F(k) = \sum_i \frac{|t_i|}{\pi} e^{-i(\phi_i + k_r r_i)} \prod_{v=x,y} \frac{\sin(k_v T_{MS}/2)}{k_v}.
\]

**APPENDIX D: CALCULATING METHODS**

Field profiles in Figs. 2(c)–2(d), 3(b)–3(d), 5(b)–5(c) in the main text are calculated via commercial software MATLAB with each unit cell of the metasurface regarded as a secondary source that can radiate a spherical wave. Based on theoretical and experimental research from other groups [6–18, 28–33, 36], the main properties of a metasurface is decided by the strength of the output light and the phase of each unit cell, despite the unit cell’s radiating type. Thus, we use a spherical wave as a secondary source to test the validity of the field profile.

Specifically, the conjugate zone in Fig. 3(d) is computed through deduction as follows:

Wavefront is the contour map of the wave’s phase, and wave vector is the gradient vector of this map, written
as \( \mathbf{k} = -\nabla \varphi \). Thus, the wave will propagate along \( \mathbf{k} \). If one want to recovery the incident wave, we can just reverse the direction of \( \mathbf{k} \) such that \(-\mathbf{k} = \nabla \varphi = -\nabla (-\varphi)\). As shown in Fig. 8(a), a plane wave is generated by a metasurface with a phase distribution of \(-0.3\varphi r\) located along \( y = 0 \). The wave propagates at \(-17.5^\circ\), as computed with \( \arcsin(-0.3) = -17.5^\circ \). Figure 8(b) is computed by reversing the phase distribution as \( 0.3\varphi r \) to rebuild the incident wave.

**APPENDIX E: DIFFRACTING PATTERNS WITH DIFFERENT VALUES OF \( T^{MS} \)**

\[
\mathcal{F}(k) = \sum_i |t_i| \sin(\frac{k T^{MS} i}{2}) e^{-i(\phi_i + k x_i)}
\]

degenerates to
\[
\mathcal{F}(k) \approx \sum_i \frac{T^{MS} i}{2\pi} e^{-i(\phi_i + k x_i)}
\]

when the width parameter \( T^{MS} \) is sufficiently small and the strength of \( \mathcal{F} \)-parameters is approximately proportional to the size of \( T^{MS} \). This also means that when \( T^{MS} \) is sufficiently small, the diffracting patterns remain the same regardless of the value of \( T^{MS} \). However, when \( T^{MS} \) is large (still smaller than a wavelength), it will affect \( \mathcal{F} \) as a sine function; the corresponding results can be seen in Fig. 6(a)–6(b). We also plotted different diffracting patterns of the designed convex-concave double lens for different \( T^{MS} \), as shown in Figs. 9(a)–9(c). The incident wavelength is \( 1 \mu m \) and the size of the unit cell is 500 nm. All the values of \( T^{MS} \) are chosen as \( T^{MS} < \Lambda = 500 \) nm, and all the diffracting patterns are almost the same in this case. As for metalenses designed in Fig. 5, \( \mathcal{F} \)-parameters differ when varying sizes of \( T^{MS} \) from 100 nm to 700 nm, as shown in Figs. 9(d)–9(f). The position of each diffractive peak remains the same, while the amplitude varies for different values of \( T^{MS} \), and this result fits with the diffracting patterns of a metasurface grating, as stated in Appendix B.

**FIG. 8: (color online) (a) A propagating plane wave and (b) rebuilt incident wave depicted in a dashed box.**

**FIG. 9: (color online) Calculated \( \mathcal{F} \)-parameters for the convex-concave double lens designed in Figs. 2–3 with (a) \( T^{MS} = 100 \) nm, (b) \( T^{MS} = 300 \) nm, (c) \( T^{MS} = 500 \) nm. Calculated \( \mathcal{F} \)-parameters for the metalenses designed in Fig. 5 with (d) \( T^{MS} = 100 \) nm, (e) \( T^{MS} = 300 \) nm, and (f) \( T^{MS} = 700 \) nm.**
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