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# On superresolution in virtual image in a transparent dielectric sphere

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Micrometer-sized lenses are known to be able to resolve objects beyond the diffraction limit. In this paper, using the matrix formalism in imaging, we discuss two possible models of this phenomenon. The first model considers the transformation of the source field keeping the real image unchanged. The second model is focused on finding the scattering matrix a particle that gives super resolution in virtual image. Both approaches demonstrate the required super resolution. Disadvantages of the proposed models and possible ways to solve them are discussed.

**Keywords:** diffraction limit, Mie theory, virtual image, superresolution, diffraction.

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## Introduction

The phenomenon of super-resolution in the virtual image using small spherical micro-lenses on the order of a few micrometers [1] has caused great interest. Confirmation of this effect has been reported in many papers [2]. At the same time, a theoretical explanation for this phenomenon is under discussion. Various models have been proposed, for example, based on the super-oscillation effect [3]. Another model relates super-resolution to the focusing of radially polarized light, which results in longitudinally polarized light at the particle exit and the corresponding overcoming of the diffraction limit [4,5]. There are models that use the whispering gallery [6] and interference [7] excitation features of modes. In general, these approaches can be divided into models based on the scattering function of a point light source [8], on a sphere, and models based on the consideration of a photon nano-jet [9]. A discussion of which model is more adequate to the experiment is available in [10].

This paper relies on a consideration of the point spread function (PSF). Many authors have noted that with this approach, the limitation imposed on the optical resolution is mainly due to the diffraction blurring of the PSF in the virtual image [6,10]. As a rule, a model of a sphere or cylinder together with the source is considered, then the diffraction problem is solved, and the PSF is constructed based on this solution. The results are unambiguously related to the properties of the scattering sphere, its size and refraction index. In most cases, this approach does not lead to a super-resolution effect [6,10].

In the present paper, the inverse problem is solved, namely, the possibility of super-resolution is considered by specifying the required PSF and determining the appropriate particle parameters and other factors.

The first part of the paper introduces a mathematical apparatus that reduces the problem to the solution of a system of linear equations. The second and third parts discuss the properties of the resulting solution: the second part discusses the possibilities associated with changing the source field, and the third part — with changing the properties of the particle. In both cases, it is possible to find the necessary solution, but there are difficulties related to its physical meaning. In addition, the problem does not have a single solution. As a result, we discuss only the possibility in principle that such solutions exist, as well as the various possibilities for enhancing the super-resolution effect.

## Matrix operator for converting a field into its optical image

According to Abbe's theory, the optical image produced by some field source is a reconstructed Fourier transform, determined by discarding the evanescent modes. Using this definition, the virtual image field is calculated [6,7,10] by the formula

$$\mathbf{E}_{\text{im}}(x, y, z) = \left(\frac{1}{2\pi k}\right)^2 \iint\limits_{k_x^2+k_y^2\le k^2} \tilde{\mathbf{E}}^*(k_x, k_y, z_0) \times e^{-i[k_x y + k_y y + k_z(z-z_0)]} dk_x dk_y. \quad (1)$$

Here, $\tilde{\mathbf{E}}$ — two-dimensional Fourier - in-plane field transform $xy$ at $z = z_0$, where $k = 2\pi/\lambda$, $k_z^2 = k^2 - k_x^2 - k_y^2$ — the corresponding wave numbers, and the asterisk indicates complex conjugation. Formula (1) can be rewritten in another form, using an integral written in ordinary coordinate space:

$$\mathbf{E}_{\text{im}} = \frac{k^2}{4\pi} \iint\limits_{\Gamma} \big(G(\mathbf{n}, \nabla)\mathbf{E}^* - \mathbf{E}^*(\mathbf{n}, \nabla)G\big) dS_0. \quad (2)$$

Here, $G = \exp[ik|\mathbf{r} - \mathbf{r}_0|]/k|\mathbf{r} - \mathbf{r}_0|$ — the Green's function of the wave equation, the operator

$$\nabla = \frac{1}{k}\left(\frac{\partial}{\partial x_0}, \frac{\partial}{\partial y_0}, \frac{\partial}{\partial z_0}\right),$$

and the integration region $\Gamma$ represents an infinite surface homotopic to the plane.

Note, that formula (1) indicates that the source field $\mathbf{E}$ cannot be uniquely reconstructed from the field $\mathbf{E}_{\text{im}}$ (because the information about the evanescent waves in (1) has been removed). However, it is possible to raise the question of obtaining additional information by imposing special conditions on the field $\mathbf{E}$ which - then. You can, for example, take into account special properties of the source or the specifics of field formation $\mathbf{E}$. In particular, this paper considers the case where the field $\mathbf{E}$ is formed by diffraction on a particle. Based on formulas (1) and (2), the solution of such an inverse problem leads to an integral equation, which presents difficulties for the corresponding analysis. The situation can be improved by introducing an operator acting on the coefficients of the source field decomposition by vector spherical functions. This approach leads to a system of linear equations. The above operator can be used to calculate the fields (1), (2) with greater accuracy than by direct numerical integration. The accuracy of calculations in this case is determined by the number of modes taken into account in the decomposition of the field by vector spherical functions.

In most cases, the source field $\mathbf{E}$ included in (1) can be represented as a decomposition of the vector spherical functions $\mathbf{M}$, $\mathbf{N}$ of the third kind. This is, for example, the scattered field in the Mie [11] theory:

$$\mathbf{E} = \sum_{l,m} a_{lm}\mathbf{N}^{(3)}_{lm} + b_{lm}\mathbf{M}^{(3)}_{lm}. \tag{3}$$

The normalization of the functions $\mathbf{M}$, $\mathbf{N}$ is the same as in [12], the angular dependence is given by $e^{im\varphi}$. The coefficients included in (3) are conveniently represented as column $\begin{pmatrix} b_{lm} \\ a_{lm} \end{pmatrix}$. The numbering of the components of this column is the same as in [13]. The image field (1), (2) is regular throughout space, and, accordingly, can be represented as a expansion in vector spherical functions of the first kind, bounded at the origin of coordinates. It is convenient to perform this decomposition by complex conjugate functions:

$$\mathbf{E}_{\text{im}} = \sum_{l,m} \tilde{a}_{lm}\mathbf{N}^{(1)*}_{lm} + \tilde{b}_{lm}\mathbf{M}^{(1)*}_{lm}. \tag{4}$$

We can introduce an image matrix operator $\mathbf{A}$, defined by the relation

$$\begin{pmatrix} \tilde{b}_{lm} \\ \tilde{a}_{lm} \end{pmatrix} = \mathbf{A} \begin{pmatrix} b^*_{\nu\mu} \\ a^*_{\nu\mu} \end{pmatrix}. \tag{5}$$

To obtain explicitly the elements of the matrix $\mathbf{A}$, it is necessary to substitute the form (3) in expression (1) and then decompose the result by vector spherical functions in the form (4). An explicit view for the components of the operator $\mathbf{A}$ and a description of the calculation method are given in the Appendix. Since the image field does not allow us to unambiguously reconstruct the source field, then

$$\det \mathbf{A} = 0. \tag{6}$$

Using definitions (1) and (2), it can be shown that for any natural number $n$, the following relation is true

$$\mathbf{A} = \frac{\mathbf{A}^n}{2^{n-1}}. \tag{7}$$

It follows from (7) that the columns of the matrix $\mathbf{A}$ are its eigenvectors with eigenvalue equal to 2. Note, that the matrix $\mathbf{A}$ has, generally speaking, infinite dimensionality, but in practical calculations it is natural to limit ourselves to a finite number of modes. It is convenient to take the number of corresponding modes in expansions (3) and (4) equal, in which case the matrix $\mathbf{A}$ becomes square. Note, that relations (6) and (7) are valid, strictly speaking, only in the limit of an infinite number of modes.

Using relation (7), we can determine the core of the operator $\mathbf{A}$. Let the matrix $\mathbf{Q}$ contain as columns the vectors from the operator core $\mathbf{A}$, then $\mathbf{AQ} = 0$. Using conditions (7), it is easy to see that in this case,

$$\mathbf{Q} = \mathbf{I} - \mathbf{A}/2. \tag{8}$$

Note that in formula (5) we introduced the operator $\mathbf{A}$, which acts on the columns of coefficients included in the expansion of the field $\mathbf{E}$ (3) by spherical functions of the third kind. In the case where the field $\mathbf{E}$ is decomposed by functions of the first kind (finite at the origin), in the formula similar to (5), the multiplier $1/2$ shall be added to the right side. This is due to the fact that spherical functions of the first kind can be represented as a half-sum of functions of the third and fourth kinds $\mathbf{M}^{(1)} = 1/2\,(\mathbf{M}^{(3)} + \mathbf{M}^{(4)})$ (a similar relation is also true for $\mathbf{N}$). From formula (2) and the Sommerfeld radiation condition for solutions at infinity, it follows that the functions of the 4-th type do not contribute to the image. Physically, this means that waves converging to the origin of coordinates simply do not reach the aperture of the optical device, because they propagate in the opposite direction.

## Super-resolution in image in transformation of source fields

According to the definition of matrix $\mathbf{Q}$, the product $\mathbf{AQ} = 0$. In this case, when transforming the field (3) in the form of

$$\mathbf{E} \to \mathbf{E} + \mathbf{QE}^{\mathrm{Q}}, \tag{9}$$

where $\mathbf{E}^{\mathrm{Q}}$ is an arbitrary vector - column, the image field (1) does not change. The situation is different in the presence of a scattering particle, such as a sphere. In this case, the $\mathbf{E}$ field can be interpreted as incident on the particle and giving a real image, which does not change when transforming (9). The transformation (9) changes the image determined by scattering on the sphere at the expense of the multiplier $\mathbf{QE}^{\mathrm{Q}}$. The field $\mathbf{E}^{\mathrm{s}}$, scattered by a particle, can be represented as

$$\mathbf{E}^{\mathrm{s}} = \mathbf{SE}, \tag{10}$$

where $\mathbf{S}$ — the scattering matrix [13]. Applying transformation (9) to $\mathbf{E}$, we find that $\mathbf{E}^{\mathrm{s}}$ converts to $\mathbf{E}^{\mathrm{s}} \to \mathbf{E}^{\mathrm{s}} + \mathbf{SQE}^{\mathrm{Q}}$. However, the product $\mathbf{ASQE}^{\mathrm{Q}}$ does not have to be zero. This makes it possible to consider a problem, in which the virtual image in the sphere changes independently of the real image obtained in the absence of the sphere. To solve such a problem, it is proposed to search for corrections to the incident field in the form $\mathbf{QE}^{\mathrm{Q}}$, where the vector $\mathbf{E}^{\mathrm{Q}}$ is unknown. In this case, we can consider a situation in which the resolution in the real image is limited by the diffraction limit, and the virtual image can give resolution beyond the diffraction limit. This is exactly the situation observed in the experiments [1].

Naturally, we are interested in $\mathbf{QE}^{\mathrm{Q}}$ corrections commensurate with the initial field $\mathbf{E}$, at least not exceeding this field by orders of magnitude. In order to meet the super-resolution and commensurability conditions of $\mathbf{QE}^{\mathrm{Q}}$ and $\mathbf{E}$, it is natural to consider the substrate on which the sphere is located. The point is that the modes included in the Mie theory sums are insufficient to form the extremely small virtual image [14]. Consider, for example, the situation with a perfectly conductive substrate. In this case, we can talk about the presence of the field scattered by the sphere and the field scattered by its image in the substrate. As a result, the scattered field comes from two centers (Fig. 1):

$$\mathbf{E}_1^{\mathrm{s}} = \mathbf{SE}, \tag{11}$$

$$\mathbf{E}_2^{\mathrm{s}} = \mathbf{RSE}. \tag{12}$$

In the figure, the origin of coordinates is chosen at the center of the real sphere. The value $\mathbf{R}$ — matrix of reflection from the substrate (in the case of a perfectly conducting substrate $\mathbf{R}$ — a diagonal matrix whose elements are equal $\pm 1$ depending on the number of the reflected mode) [15]. Strictly speaking, in the presence of a substrate, $\mathbf{S}$ should be understood as the scattering matrix of the particle on the substrate [15]. We use a simplified model in which the matrix $\mathbf{S}$ is defined by the Mie theory. The field $\mathbf{E}_1^{\mathrm{s}}$ comes from the center of the real sphere, and the field $\mathbf{E}_2^{\mathrm{s}}$ — from the center of its reflection in the substrate. Accordingly, the image field can be represented as a two-center decomposition. Given transformation (9), we can write

$$\mathbf{E}_1^{\mathrm{im}} = \mathbf{A}(\mathbf{SE} + \mathbf{SQE}^{\mathrm{Q}} + \mathbf{E}), \tag{13}$$

$$\mathbf{E}_2^{\mathrm{im}} = \mathbf{A}(\mathbf{RSE} + \mathbf{RSQE}^{\mathrm{Q}}). \tag{14}$$

Here, it is taken into account that $\mathbf{AQ} = 0$. Formulas (13), (14) are a system of equations to determine $\mathbf{E}^{\mathrm{Q}}$.

The field decomposition in Mie theory considers a finite number of L [16] modes. In this case, conditions (13), (14) represent a system of linear equations in which the number of unknowns is half the number of equations. In reality, half of these equations can be discarded due to their linear dependence.

As noted above, the columns of the matrix $\mathbf{A}$ are its eigenvectors. Given the explicit form of the column elements and condition (7), we can state that all even columns are expressed through odd columns and vice versa. The same remark is true for strings (this is essentially what causes the equality $\det\mathbf{A} = 0$). It follows that in conditions (13) and (14), even (or odd) lines can be crossed out, since they are defined by odd (or even) lines.

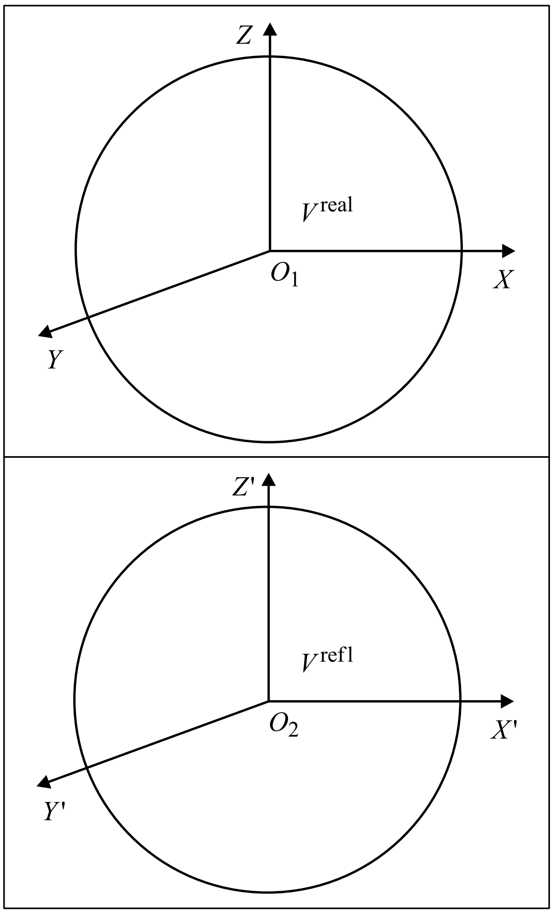


**Figure 1.** Schematic images of the sphere on the substrate and its mirror reflection. The vector $\mathbf{E}_1^{\mathrm{s}}$ contains the expansion coefficients relative to the center of the real sphere $O_1$, and the vector $\mathbf{E}_2^{\mathrm{s}}$ relative to the center of the reflected sphere $O_2$.

By discarding half of the lines in each of the relations (13), (14), the system is converted to a quadratic system: the number of equations equals the number of unknowns. However, the system still has no solution because the matrix $\mathbf{Q}$ is degenerate similarly $\mathbf{A}$ in the $\mathbf{QE}^{\mathrm{Q}}$ corrections. Because the determinant of the resulting system is zero, and the system has no solutions. If we look for corrections in an arbitrary form, we lose the invariance of the actual image.

In order to arrive at a single-valued solution, it is necessary to reduce the dimensionality of the system. For this purpose, only even or odd columns can be selected in the matrix $\mathbf{Q}$. As a result, we again arrive at an overdetermined system in which the number of equations is twice the number of unknowns. Although it is not possible to reduce the number of equations further by

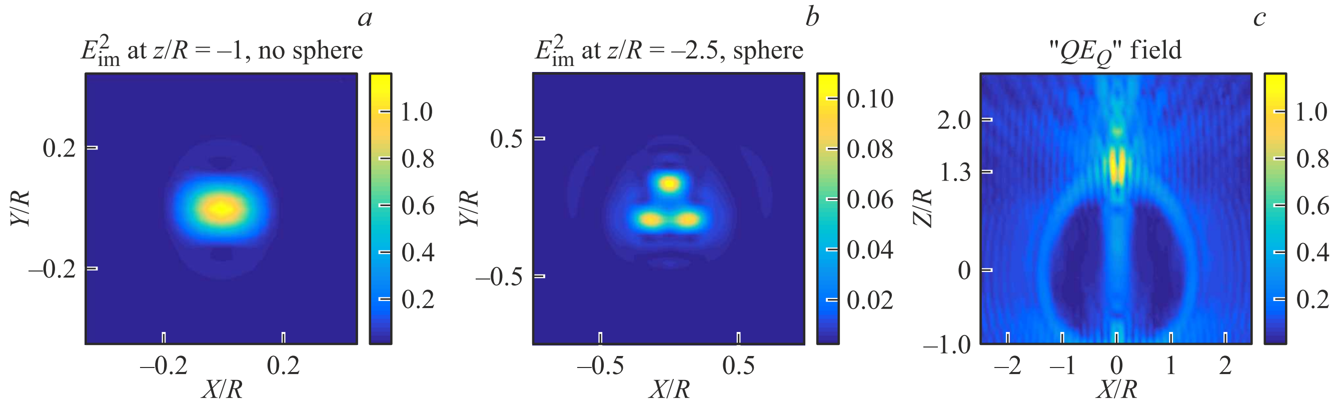


**Figure 2.** ($a$) Real image in the source plane without a sphere; ($b$) virtual image in the presence of a sphere; ($c$) module „additional“$\mathbf{E}^{\mathrm{Q}}$, which can be interpreted as a field that exists in the absence of a sphere. The latter distribution has some „chaotic“ character, which in no way indicates the presence of sources in the $z = -R$ plane. In this calculation the sphere is located on a perfectly conducting substrate, the parameters of the sphere are $2\pi R/\lambda = 24.5$, $n = 1.46$.

crossing out the lines, the analysis shows that the problem can be overcome by simply abandoning condition (13). This is possible for several reasons. Firstly the virtual image field given by the $\mathbf{A}(\mathbf{SE} + \mathbf{E})$ summand is concentrated predominantly below the substrate in the reflected sphere volume $V^{\mathrm{refl}}$ (Fig. 1). Therefore, the corresponding vector can be transformed through the reflected basis without loss of accuracy, using only $L$ mode. This circumstance allows us to exclude the contribution of this summand in the virtual image field. As the calculation shows, the modes $\mathbf{Q}$ give an order of magnitude greater contribution to the image field in the value of the summand $\mathbf{RSQE}^{\mathrm{Q}}$ than in the value of the summand $\mathbf{SQE}^{\mathrm{Q}}$, which leads only to „small“ distortions of the image field. These distortions are predominantly localized in the volume of the real sphere $V^{\mathrm{refl}}$ (Fig. 1). Physically, this means that the rays reflected from the sphere and the substrate contribute an order of magnitude more to the image than the rays that have passed through the sphere.

The field $\mathbf{E}_2^{\mathrm{im}}$ cannot be uniquely defined. We propose to describe this field as

$$\mathbf{E}_2^{\mathrm{im}} = -1/2\mathbf{A}\mathbf{T}_{12}\mathbf{A}(\mathbf{SE} + \mathbf{E}) + \mathbf{AE}^{\mathrm{supres}}. \qquad (15)$$

Here, $\mathbf{T}_{12}$ — the transformation matrix of spherical modes of the first kind from real to reflected sphere. The first summand is chosen so as to zero out the image that the real sphere gives without taking into account the small contribution of mod $\mathbf{E}^{\mathrm{Q}}$. The second summand in (15) $\mathbf{AE}^{\mathrm{supres}}$ describes the virtual image that provides super-resolution.

Here is an example. Consider three dipoles located at the vertices of a right triangle with side $\lambda/8$, in plane $z = -R$, where $R$ — radius of sphere. The corresponding field $\mathbf{E}$ can be interpreted as the result of a plane wave passing through three small holes in an opaque screen. The result of the calculations is shown in Fig. 2.

The physical explanation of the super-resolution phenomenon in Fig. 2 is related to the diffraction of evanescent waves on the sphere. As a result of diffraction, evanescent waves are converted into propagating waves. In the absence of a sphere, the microscope aperture does not interact in any way with the evanescent components. The spherical particle thereby transmits information about the near field, with the reflection from the substrate actually making the main contribution.

We realize that the proposed approach is not yet a theory, but some „leading considerations“. Firstly, the field structure $\mathbf{E}$ is determined by Maxwell's equations, not by the presence of super-resolution in the virtual image. Secondly, the distribution of the additional field $\mathbf{QE}^{\mathrm{Q}}$ (Fig. 2, $c$) is not localized near the dipoles, but has maximums at a considerable distance from the substrate. The interpretation with the diffraction of evanescent waves on the sphere actually relies on the choice of the field $\mathbf{E}_2^{\mathrm{im}}$ in formula (15).

The particular form of the field $\mathbf{QE}^{\mathrm{Q}}$, strictly speaking, depends on the truncation procedure of equations (13), (14), and on the choice of fields $\mathbf{E}_1^{\mathrm{im}}$ and $\mathbf{E}_2^{\mathrm{im}}$. It is not clear whether these conditions can be formulated to localize the $\mathbf{QE}^{\mathrm{Q}}$ field near the substrate?

## Building a super-resolution particle scattering matrix

To construct the theory without changing the incident field, one shall find a scattering matrix $\mathbf{S}$, which provides super-resolution in the virtual image. The appearance of this matrix depends on how the corresponding point sources are considered. The decomposition of the point source field in the near and far zones is different [17]. The scattering matrix $\mathbf{S}$ acts to decompose the sources in the near zone, assuming the sources are outside the particle. When constructing the scattering matrix $\mathbf{S}$, we will proceed from relations (13), (14). Let even components of the vector $\mathbf{E}_{1/2}^{\mathrm{im}}$ contain even components of the difference $\mathbf{E}_1^{\mathrm{im}} - \mathbf{AE}$, and

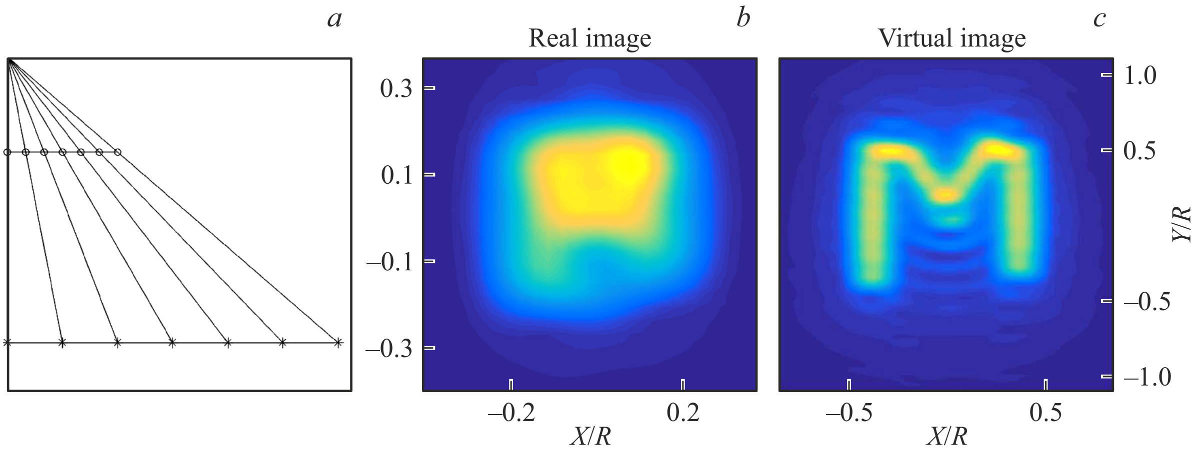


**Figure 3.** (*a*) Schematic representation of the source positions (circles) and their enlarged images (asterisks).(*b*) Image of a letter „M" of order $\lambda$ in free space (indistinguishable due to diffraction limit).(*c*) The same is in the action of the scattering matrix. For the construction the point sources were placed along the contours of the letter „M" with $x$- polarization. The value $R$ is the same as in Fig. 2.

odd components $\mathbf{E}^{\mathrm{im}}_{1/2}$ contain odd components $\mathbf{E}^{\mathrm{im}}_{2}$. You can also construct a matrix $\mathbf{A}^{\mathrm{im}}_{\mathrm{R}}$, whose even lines are equal to the even lines of matrix $\mathbf{A}$ and whose odd lines — the odd lines of the product $\mathbf{A}\,\mathbf{R}$. Then relations (13), (14) can be written as

$$\mathbf{E}^{\mathrm{im}}_{1/2} = \mathbf{A}^{\mathrm{im}}_{\mathrm{R}}\mathbf{S}\,\mathbf{E}. \tag{16}$$

If the vectors $\mathbf{E}$ form a matrix $\mathbf{X}$ and the vectors $\mathbf{E}^{\mathrm{im}}_{1/2}$ — a matrix $\mathbf{Y}$, then the equation connecting them can be written as $\mathbf{Y} = \mathbf{A}^{\mathrm{im}}_{\mathrm{R}}\mathbf{S}\mathbf{X}$. From this it is easy to find a solution for the matrix $\mathbf{S}$:

$$\mathbf{S} = (\mathbf{A}^{\mathrm{im}}_{\mathrm{R}})^{-1}\mathbf{Y}\mathbf{X}^{-1}. \tag{17}$$

If the position of the sources $\mathbf{E}$ is wrong, the determinant of the matrix $\mathbf{X}$ may be zero. Therefore, it is necessary to ensure that the vector $\mathbf{E}$ is not zero, and that the vectors $\mathbf{E}$ themselves are linearly independent. If one searches the matrix $\mathbf{S}$ diagonally along the azimuthal modes, the source positions can be chosen along one straight line. Preferably, the matrix $\mathbf{X}$ and $\mathbf{Y}$ respectively contain sources with different polarization, in which case the resolution in the virtual image is independent of the polarization.

It might seem that a matrix $\mathbf{S}$ would give super-resolution only for sources along this straight line. However, this is not the case because similar sources along other directions are linearly dependent. Thus, a rotation of the source position by a certain angle will be accompanied by a rotation of the image by a similar angle. Moreover, as the calculations show, the matrix $\mathbf{S}$ will produce an image even if the sources are placed between the positions that were chosen to construct the matrix $\mathbf{X}$ (Fig. 3).

The image in Fig. 3, *c* shows the matrix $\mathbf{S}$, which provides super-resolution. At the same time, the elements of the matrix $\mathbf{S}$ are too large, of the order $10^{15}$. Although we have not yet been able to find a scattering matrix whose elements would have realistic values, we do not rule out the existence of such a matrix.

In principle, this problem is partially solved by reducing the dimensionality of the matrices $\mathbf{X}$, $\mathbf{Y}$ (i. e., selecting conditions of smaller dimensionality of the desired matrix $\mathbf{S}$). In this case, the matrix itself $\mathbf{S}$ is determined from relations (13), (14) in an ambiguous way. This approach, in principle, allows us to obtain a scattering matrix $\mathbf{S}$ with elements of the order of unity, but only for the first azimuthal modes $m = 1, 2, 3$. For higher modes, it is not possible to get rid of large values of matrix elements $\mathbf{S}$. For high $m$, the matrix elements $\mathbf{Y}$ are several orders of magnitude larger than those of matrix $\mathbf{X}$. This is due to the fact that the virtual image is localized at a much greater distance from the origin than the position of the source. It is possible to get rid of the large scattering matrix elements by choosing $\mathbf{Y}$ so that the image represents a localized bright point, but the columns of the matrix $\mathbf{Y}$ will be of the same order as the columns of the matrix $\mathbf{X}$.

## Conclusion

We know of no observations of super-resolution in virtual imaging using dielectric spheres in the absence of a substrate. This paper shows that the super-resolution is caused by the substrate no less than by the sphere itself. We have considered two models of super-resolution theory. The first relies on the transformation of the source field, in which their actual image does not change because of the presence of a sphere. The second is based on the construction of a scattering matrix giving super-resolution in the virtual image. Although super-resolution has been studied experimentally in many papers [2], a unified theory of this phenomenon has not yet been created. The models we offer are not free from disadvantages either. In the first model, it is difficult to interpret the mathematical results and the possibility of direct experimental verification.

In the second — the obtained solution also does not have a clear physical meaning, but represents a possible mathematical interpretation of the phenomenon. In any case, it seems important to us to investigate the various models that lead to super-resolution in terms of testing new ideas.


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### Conflict of interest

The author declares that he has no conflict of interest.

## Appendix

To calculate the operator **A**, we used the expansion of a plane wave with an arbitrary direction of the wave vector and polarization [12]. It is convenient to calculate the arising integrals by first converting them to the polar coordinate system in the space of wave vectors. In this case, we actually have to calculate decompositions (4) for each of the modes **M** and **N**. The corresponding decomposition for **M** has the form

$$\mathbf{E}_{\text{im}}(\mathbf{M}_{\nu\mu}) = \sum_{l,m} d_{lm}^{\nu\mu}\mathbf{N}_{lm}^{(1)^*} + c_{lm}^{\nu\mu}\mathbf{M}_{lm}^{(1)^*}. \tag{18}$$

The decomposition for the functions **N** is similar to (18) and differs only by swapping the coefficients $c$ and $d$, which follows from the relation $\mathbf{N} = \text{rot}(\mathbf{M})/k$. Calculating the integrals over the „angle" variable, we arrive at the following form for the coefficients:

$$\begin{aligned} d_{lm}^{\nu\mu} = \frac{4\pi\gamma_{lm}(-i)^{l-\nu}\delta_{m\mu}}{2l(l+1)} \int_0^1 \Big\{ & -\text{sign}(m)P_\nu^{(|m|+1)} \\ & \times \left[|m|\sqrt{1-t^2}P_l^{|m|} + tP_l^{(|m|+1)}\right] + \text{sign}(m)(\nu+|m|) \\ & \times (\nu-|m|+1)P_\nu^{(|m|-1)}\left[|m|\sqrt{1-t^2}P_l^{|m|} + (l+|m|)\right. \\ & \left.\times (l-|m|+1)tP_l^{(|m|-1)}\right] - mP_\nu^{(|m|)}\left[P_l^{|m|+1} - (l+|m|)\right. \\ & \left.\times (l-|m|+1)P_l^{(|m|-1)}\right]\sqrt{1-t^2}\Big\}dt, \end{aligned} \tag{19}$$

$$\begin{aligned} c_{lm}^{\nu\mu} = \frac{4\pi\gamma_{lm}(-i)^{l-\nu}\delta_{m\mu}}{l(l+1)} \int_0^1 \Big\{ & \frac{1}{2}P_\nu^{|m|+1}P_l^{|m|+1} \\ & + \frac{1}{2}(\nu+|m|)(\nu-|m|+1)(l+|m|)(l-|m|+1) \\ & \times P_\nu^{|m|-1}P_l^{|m|-1} + m^2 P_\nu^{(|m|}P_l^{|m|}\Big\}dt, \end{aligned} \tag{20}$$

here and hereafter, in all cases the argument of the Legendre polynomials is $t$, i.e. $P_l^{|m|} = P_l^{|m|}(t)$. Formulas (19) and (20) are valid at $\mu \neq 0$. If $\mu \equiv 0$ the corresponding formulas take the form of

$$d_{lm}^{\nu\mu} \equiv 0, \tag{21}$$

$$c_{lm}^{\nu\mu} = \frac{4\pi\gamma_{lm}(-i)^{l-\nu}\delta_{m\mu}}{l(l+1)} \int_0^1 P_\nu^1 P_l^1 dt. \tag{22}$$

Here, the coefficient $\gamma_{lm}$ is defined by the formula

$$\gamma_{lm} = \frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l-|m|)!}. \tag{23}$$

The complexity of calculating the integrals included in (19), (20) is mainly due to the fact that they integrate from 0 to 1, while the Legendre polynomials are orthogonal on the interval from −1 to 1. In the end, the calculation is reduced to the calculation of integrals of the form

$$I_{l\nu}^m = \int_0^1 P_\nu^{|m|}P_l^{|m|}dt. \tag{24}$$

The integral (24) can be calculated in various ways. In the case of $(-1)^{l+\nu} = 1$, the calculation is done elementarily by reducing to an integral within −1 to 1:

$$\begin{aligned} I_{l\nu}^m &= \int_0^1 P_\nu^{|m|}P_l^{|m|}dt = \frac{1}{2}\int_{-1}^1 P_\nu^{|m|}P_l^{|m|}dt \\ &= \frac{\delta_{1\nu}}{(2l+1)}\frac{(1+|m|)!}{(1-|m|)!}, \qquad (-1)^{l+\nu} = 1. \end{aligned} \tag{25}$$

In the case of $(-1)^{l+\nu+1} = 1$ we should use integration by parts, and for (24) we finally get

$$I_{l\nu}^{m} = \frac{(-1)^{\nu+(l+\nu-1)/2}}{2^l l! 2^\nu \nu!}$$
$$\times \sum_{n=1}^{\nu+m+1} \frac{l!(l+m-n)!}{((l+m-n)/2)!((l-m+n)/2)!}$$
$$\times \sum_{k=0}^{\nu} C_\nu^k C_{z-1}^{2k-\nu-m} C_m^{(n-1-2k+\nu+m)/2}(2k)!$$
$$\times (n-1-2k+\nu+m)!, \qquad (-1)^{l+\nu+1} = 1. \tag{26}$$

The summands containing negative or half-integer values of the factorial should be assumed to be zero, and as $m$ we should take the modulus, i.e. $m \geq 0$. In addition, we will assume that $l > \nu$, otherwise the indices should be reversed in expression (26).

In the result, for coefficients (19) and (20) at $\mu \neq 0$, we get

$$d_{lm}^{\nu\mu} = \frac{4\pi\gamma_{lm}(-i)^{l-\nu}\delta_{m\mu}}{2l(l+1)} \Bigg\{ -\mathrm{sign}(m)\big[(l-|m|)I_{l+1\nu}^{m+1}$$
$$+ (l+|m|+1)I_{l-1\nu}^{m+1}\big]/(2l+1) + \mathrm{sign}(m)(\nu+|m|)$$
$$\times (\nu-|m|+1)(l+|m|)(l-|m|+1)\big[(l-|m|+2)$$
$$\times I_{l+1\nu}^{|m|-1} + (l+|m|-1)I_{l-1\nu}^{|m|-1}\big]/(2l+1) + \frac{2m}{2\nu+1}$$
$$\times \big[\nu(\nu-|m|+1)I_{l\nu+1}^{m} - (\nu+|m|)(\nu+1)I_{l\nu-1}^{m}\big]$$
$$- \frac{2m}{2l+1}\big[(l+|m|)(l+1)I_{l-1\nu}^{m} - l(l-|m|+1)I_{l+1\nu}^{m}\big] \Bigg\}, \tag{27}$$

$$c_{lm}^{\nu\mu} = \frac{4\pi\gamma_{lm}(-i)^{l-\nu}\delta_{m\mu}}{l(l+1)} \Bigg\{ \frac{1}{2} I_{l\nu}^{m+1} + \frac{1}{2}(\nu+|m|)$$
$$\times (\nu-|m|+1)(l+|m|)(l-|m|+1)I_{l\nu}^{m-1} + m^2 I_{l\nu}^{m} \Bigg\}, \tag{28}$$

(In this expression, we have converted the factor $d_{lm}^{\nu\mu}$). Similarly, for the case of $\mu = 0$, we obtain

$$d_{lm}^{\nu\mu} \equiv 0, \tag{29}$$

$$c_{lm}^{\nu\mu} = \frac{4\pi\gamma_{lm}(-i)^{l-\nu}\delta_{m\mu}}{l(l+1)} I_{l\nu}^{1}. \tag{30}$$

With $(-1)^{l+\nu+1} = 1$, it is easy to show that $d_{lm}^{\nu\mu} \equiv 0$ for all $\mu$, i.e.

$$d_{lm}^{\nu\mu} \equiv 0, \quad (-1)^{l+\nu+1} = 1. \tag{31}$$

Using the expression for the coefficients $c$ and $d$, the matrix $\mathbf{A}$ in expression (5) can finally be represented as

$$\mathbf{A} = \begin{pmatrix} c_{lm}^{\nu\mu} & d_{lm}^{\nu\mu} \\ d_{lm}^{\nu\mu} & c_{lm}^{\nu\mu} \end{pmatrix}. \tag{32}$$

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