Equivalent medium theory of layered sphere particle with anisotropic shells

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\textbf{A B S T R A C T}

Researches on the optical properties of small particle have been widely concerned in the atmospheric science, astronomy, astrophysics, biology and medical science. This paper provides an equivalent dielectric theory for the functional graded particle with anisotropic shells, in which inhomogeneous and anisotropic particle was equivalently transformed into a new kind of homogeneous, continuous and isotropic sphere with same size but different permittivity, and then greatly simplify the calculation process of particle’s optical property. Meanwhile, the paper also discusses whether the charge on the particle can change the expression of its equivalent permittivity or not. These results proposed in this paper can be used to simulate the electrical, optical properties of layered sphere, it also meet the research requirement in the design of functional graded particles in different subjects.

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1. Introduction

Estimation and simulation of the optical properties for small particles became a common research subject in the atmospheric science, astronomy, astrophysics, biology, medical science and the chemistry. Because of its complexities in particle shapes and structures [1,2], several methods to resolve the problem have been suggested, for example, Rayleigh approximation [3], Lorenz–Mie theory [3,4], N-layered Mie theory [5–8], DDA [9,10], T-matrix method [11–16], Separation of Variables Method [2,17], FDTD [18,19], Deby series solution [20–22] etc. Besides, because of its clear physical significance and concision, equivalent medium theory has been obtained much attention, and it has been used to do some numerical simulation works on the optical and electrical properties of intermixed random medium [23,24]. With the help of the equivalent medium theory, Videen et al. discussed the electromagnetic scattering of sphere with an absorptive core [25]. Kolokolova et al. simulated the electromagnetic scattering property of discontinuous particle, and compared it with the experiment results [26]. They found that the equivalent medium theory does not work for calculations of back-scattering characteristics of large particles. Li et al. proposed the equivalent permittivity of a multilayered sphere, and discussed its application in the calculation of particles’ electromagnetic scattering [27]. They found the equivalent permittivity can be used when the Rayleigh hypothesis is meet. Liu et al. compared the similarities and differences of four major theories on the equivalent medium, such as the Bruggeman theory, the Maxwell-Garnett theory, and two different Wiener bounds, and analyzed their scopes of application in

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calculating the electromagnetic scattering properties of inhomogeneous medium particles [28].

However, these models mentioned above are only applicable to the isotropic medium. Meanwhile, functional graded materials make it easy to achieve invisibility at specific frequency ranges, which is attracting more and more attentions from scientific researchers [29,30]. The anisotropic shell can significantly change the electric field distribution inside the particle, so as to realize some interesting features [29]. Numerical simulations of the electromagnetic field both inside and outside of the particle with different structural can give an important guidance to the structural designs, and the equivalent medium theory can significantly simplify related calculations and meet the accurate requirement of engineering design. There are quite a few researches on the optical properties of particles with multilayered structures or some anisotropic shells, but there is still a lack of detailed and systematic research on its equivalent permittivity. Therefore, this paper devoted to the study of equivalent permittivity of these kinds of particles with similar structures. In addition, we also discussed the influences of the surface charge on the particle’s equivalent permittivity.

2. Basic theories and models

2.1. Equivalent permittivity of homogeneous particle with some anisotropic shells

Assuming there’s a core–shell structured spherical particle with an anisotropic coating, and the core is an isotropic medium, its permittivity is \( \varepsilon_0 \) and the radius is \( r_0 \). The shell is an anisotropic material, its outer radius is \( r_1 \), and its permittivity can be expressed with the spherical coordinate as follows.

\[
\varepsilon_s = \begin{bmatrix}
\varepsilon_r & 0 & 0 \\
0 & \varepsilon_\theta & 0 \\
0 & 0 & \varepsilon_\phi
\end{bmatrix}
\]

(1)

The background medium around the particle is isotropic and its permittivity is \( \varepsilon_b \). Considering the electrostatic field component of the incident wave is \( \mathbf{E}_{in} = \mathbf{E}_0 \mathbf{x} \). With the spherical coordinates \((r, \theta, \phi)\), the electric potentials both inside of the particle and outside of it can be expressed as [29,30],

\[
\begin{align*}
\phi_c &= -E_r \cos \theta \quad r < r_0 \\
\phi_s &= (A_1 r^{t_1} + A_2 r^{t_2}) \cos \theta \quad r_0 < r < r_1 \\
\phi_h &= (-r + D/r^2) E_0 \cos \theta \quad r > r_1
\end{align*}
\]

(2a)

(2b)

(2c)

\[ t_{1,2} = \left( -1 \pm \sqrt{1 + 8\varepsilon_0/\varepsilon_r} \right) / 2, \]
\[ E_0 \] is the intensity of electrostatic field, and \( A_1, A_2, E_c, D \) are undetermined coefficients, which can be determined through the corresponding boundary conditions,

\[
\begin{align*}
\begin{cases}
\phi |_{r = r_0} = \phi_c = \phi_s \quad &\varepsilon_0 \frac{\partial \phi_r}{\partial r} = \varepsilon_r \frac{\partial \phi_s}{\partial r} \\
\phi |_{r = r_1} = \phi_c = \phi_h \quad &\varepsilon_0 \frac{\partial \phi_r}{\partial r} = \varepsilon_r \frac{\partial \phi_h}{\partial r}
\end{cases}
\end{align*}
\]

(3)

Through Eqs. (2), (3) we can obtain

\[
E_c = \frac{3\varepsilon_c \varepsilon_b (t_2 - t_1) E_0}{(\varepsilon_r t_2 - \varepsilon_b) \Delta t_1 - (\varepsilon_r t_1 - \varepsilon_b) \Delta t_2}
\]

(4)

\[
A_1 = -\frac{(\varepsilon_r t_2 - \varepsilon_b) E_c}{\varepsilon_r (t_2 - t_1) t_1 - 1} \quad A_2 = \frac{(\varepsilon_r t_1 - \varepsilon_b) E_c}{\varepsilon_r (t_2 - t_1) t_1 - 1}
\]

\[
D = \frac{\varepsilon - \varepsilon_b}{\varepsilon + 2\varepsilon_b} r_0^3
\]

Here

\[
a_{t,2} = (\varepsilon_r t_1 + 2\varepsilon_b) \lambda_{t,2}^{t_1}, \lambda = r_1/r_0, a_{t,2} = (\varepsilon_r t_1 + 2\varepsilon_b) \lambda_{t,2}^{t_1-1}
\]

\[
\frac{\varepsilon}{(\varepsilon_r t_2 - \varepsilon_b) \lambda_{t,2}^{t_1-1}} - \frac{\varepsilon}{(\varepsilon_r t_1 - \varepsilon_b) \lambda_{t,2}^{t_1-1}}
\]

(5)

Compared (2c) with the expression of outer potential for a homogeneous sphere in a uniform electric field, \( \varepsilon \) can be considered as the equivalent permittivity of spherical particle with an anisotropic coating. As shown in the above equation, the coefficient before \( E_0 \) in \( E_c \) is a constant, which related to the core–shell radius ratio and the permittivity of the particle, which means that the core–shell geometric parameters and the electrical properties of shell all can change the electric field in the particle.

Based on the new parameter expression \( \varepsilon \), the equivalent dielectric constant of the coated sphere with an anisotropic shell, and the method proposed by Li et al. [27], we can expand this result to other conditions, and then obtain the equivalent parameter of any particle with some types of special structures. Those results are discussed as follows.

1) \( N \)-layered core–shell particle with an anisotropic shell and \( N - 1 \) isotropic shells

For this kind of special particle, supposed the radius for the core and shells are \( r_0, r_1, r_2, r_3, \ldots, r_N \), the permittivity is \( \varepsilon_0, \varepsilon_1, \varepsilon_2, \varepsilon_3, \ldots, \varepsilon_N \), respectively. Here the dielectric constant \( \varepsilon_1 \) for the first shell have a similar expression with the Eq. (1). In order to obtain the equivalent permittivity of this multi-layered particle, we can set the core and the first shell as a new core, whose dielectric constant can be obtained through the Eq. (5). With a similar operation with reference [27] we can obtain its permittivity.

\[
\varepsilon_n = \frac{\beta_n + 2\varepsilon_n}{\beta_n + 2\varepsilon_n - \varepsilon_0} \varepsilon_0 \quad \text{sign as} \quad \beta_n \varepsilon_n
\]

Here,

\[
\delta_n = r_0^{3}\frac{\gamma_n}{\gamma_{n-1}}, \varepsilon_n = \varepsilon_0/\varepsilon_{n-1}, \beta_n = 1, \beta_1 = \varepsilon, \
\]

\[
\beta_n = \frac{(\beta_{n+1} + 2\varepsilon_n)}{(\beta_{n+1} + 2\varepsilon_n) - \varepsilon_0} \varepsilon_0 \quad n = 2, 3, \ldots, N.
\]

The parameter \( E_c \) in the electric potential of the core–zone can be expressed as,

\[
E_c = \frac{3\varepsilon_c \varepsilon_b (t_2 - t_1) A E_0}{(\varepsilon_r t_2 - \varepsilon_b) \Delta t_1 - (\varepsilon_r t_1 - \varepsilon_b) \Delta t_2}
\]

(7)

\[
A = \prod_{i=2}^{N} \frac{9\varepsilon_i \varepsilon_j}{(\varepsilon_i + 2\varepsilon_b)(\varepsilon_{i-1} + 2\varepsilon_i) + 2\delta_i (\varepsilon_i - \varepsilon_b)(\varepsilon_{i-1} - \varepsilon_i)}
\]

(8)
The above equation reflects the effect of shells on particle’s inner potential.

2) N-layered core–shell particle with \( N – 1 \) anisotropic shells

For this kind of particle, supposed the radius for the core and those of the shells for the particle are \( r_0, r_1, r_2, r_3, \cdots \) \( r_N \), the permittivity for the shell is \( \varepsilon_i^1, \varepsilon_i^0, i = 2, 3, \cdots, N \), respectively. The dielectric constant of the core zone is \( \varepsilon_0 \). In order to obtain the equivalent permittivity of this particle, we firstly set \( \varepsilon_i^1 = \varepsilon_r, \varepsilon_i^0 = \varepsilon_0 \), and take the core and the first shell as a new core, whose equivalent permittivity is shown in the Eq. (6), then with a similar operation with the reference [27], we can obtain the permittivity of this particle.

\[
\varepsilon_n = \left( \varepsilon_i^0 \varepsilon_i^1 \right) \left( \frac{\varepsilon_i^0 + \varepsilon_i^1}{2} \right)^2 \left( \frac{\varepsilon_i^0 + \varepsilon_i^1}{2} \right) - \left( \frac{\varepsilon_i^0 - \varepsilon_i^1}{2} \right)^2 \left( \frac{\varepsilon_i^0 - \varepsilon_i^1}{2} \right) \varepsilon_i^0 \varepsilon_i^1
\]

here \( n = 2, 3, \cdots, N \), \( r_{11} = \left( \frac{i + 1}{i} \right) r_0 \), \( \delta_n = r_n - r_{n-1} \).
The expansion coefficient of electric potential in the core zone can be expressed as follow:

\[
E_c = \left\{ \frac{\varepsilon_i^0 \varepsilon_i^1 \left( \varepsilon_i^0 + \varepsilon_i^1 \right)^2 \left( \frac{\varepsilon_i^0 + \varepsilon_i^1}{2} \right)^2 - \left( \frac{\varepsilon_i^0 - \varepsilon_i^1}{2} \right)^2 \left( \frac{\varepsilon_i^0 - \varepsilon_i^1}{2} \right) \varepsilon_i^0 \varepsilon_i^1}{\left( \varepsilon_i^0 + \varepsilon_i^1 \right) \left( \frac{\varepsilon_i^0 + \varepsilon_i^1}{2} \right)^2 - \left( \frac{\varepsilon_i^0 - \varepsilon_i^1}{2} \right)^2 \left( \frac{\varepsilon_i^0 - \varepsilon_i^1}{2} \right) \varepsilon_i^0 \varepsilon_i^1} \right\} E_0
\]

Here \( a_{t1} = \left( \varepsilon_i^0 \varepsilon_i^1 + 2 \varepsilon_h \right) \delta_n^{-1} \).

3) N-layered core–shell particle, and the properties of shells periodic changed

For the particle, supposed its core is an isotropous medium, its permittivity and radius are \( \varepsilon_0 \) and \( r_0 \), and the odd layers are anisotropic media, their corresponding permittivity and radius are \( \varepsilon_i^1, r_i \), \( i = 1, 3, 5, \cdots \), while the even layers are isotropous media, of which the permittivity and radius is \( \varepsilon_i^0 = \varepsilon_0, r_i = 2, 4, 6, \cdots \) respectively. Then its equivalent permittivity is,

\[
e_{2n} = \frac{\beta_{2n-1} + 2g_{2n}}{\beta_{2n-1} + 2g_{2n}} + 2\beta_{2n} \varepsilon_{2n} \varepsilon_{2n}
\]

\[
e_{2n+1} = \frac{\beta_{2n-1} + 2g_{2n} \varepsilon_{2n} \varepsilon_{2n}}{\beta_{2n-1} + 2g_{2n} \varepsilon_{2n} \varepsilon_{2n}} - \frac{\beta_{2n} \varepsilon_{2n} \varepsilon_{2n}}{\beta_{2n} \varepsilon_{2n} \varepsilon_{2n}}
\]

The expansion coefficient of the inner potential in core area is

\[
E_c = \left\{ \frac{\varepsilon_i^0 \varepsilon_i^1 \left( \varepsilon_i^0 + \varepsilon_i^1 \right)^2 \left( \frac{\varepsilon_i^0 + \varepsilon_i^1}{2} \right)^2 - \left( \frac{\varepsilon_i^0 - \varepsilon_i^1}{2} \right)^2 \left( \frac{\varepsilon_i^0 - \varepsilon_i^1}{2} \right) \varepsilon_i^0 \varepsilon_i^1}{\left( \varepsilon_i^0 + \varepsilon_i^1 \right) \left( \frac{\varepsilon_i^0 + \varepsilon_i^1}{2} \right)^2 - \left( \frac{\varepsilon_i^0 - \varepsilon_i^1}{2} \right)^2 \left( \frac{\varepsilon_i^0 - \varepsilon_i^1}{2} \right) \varepsilon_i^0 \varepsilon_i^1} \right\} E_0
\]
of wind-blown sand and make it to be more reasonable and
sophisticated. Bohren and Huffman are the first one
who made theoretical analysis on the influence of
electric charge on the particle’s optical properties [34], but
they did not make any numerical analysis. In order to explain
the phenomenon that the actual measurements of micro-
wave attenuation in sand storms are much bigger than the
theoretically estimated values, and considering the charge
on particle surface, Zhou et al. used Rayleigh approxima-
tion to discuss the influences of electric charges on parti-
cles’ optical properties [35], and their studies firstly
revealed the important impact of electric charges on the
particle’s optical properties. After that, many scholars
carried out some numerical studies on the electromagnetic
scatterings of the isotropic charged sphere with different
material components [5,36–43]. However, there are still
few of researches on the electromagnetic scattering of
charged anisotropic particle [42]. In view of the diversity of
class properties in the nature, and the conviction of
using equivalent medium theory to compute particle’s
optical properties, in this section, we devoted to study the
equivalent permittivity of partially charged particles
with anisotropic shells.

Regarding to a small-sized coated sphere with local
el-ectrification, its structure and the physical parameters
are the same as them described in Section 2.1, but its
surface is partially charged, and the charge uniformly
 distributes on a spherical crown with an angle 2θ0
According to existed reference [35], the electric potential
both inside of the charged particle and outside of it should
be expressed as follows,

\[ \phi_c = -E_c r \cos \theta + A \quad r < r_0 \]  
(14a)

\[ \phi_s = B + \frac{C}{r} + (A_1 r_1 + A_2 r_2) \cos \theta \quad r_0 < r < r_1 \]  
(14b)

\[ \phi_h = \frac{D}{r} + \left( -r + E/r^2 \right) E_0 \cos \theta \quad r > r_1 \]  
(14c)

The corresponding boundary conditions are [42]:

\[
\begin{align*}
  & r = r_0 \quad \phi_c = \phi_s, \quad \varepsilon_{c,0} \frac{\partial \phi_c}{\partial r} = \varepsilon_{s,0} \frac{\partial \phi_s}{\partial r} = 0 \\
  & r = r_1 \quad \phi_c = \phi_h, \quad \varepsilon_{c,0} \frac{\partial \phi_c}{\partial r} - \varepsilon_{h,0} \frac{\partial \phi_h}{\partial r} = \sigma \mathcal{H}(\theta - \theta_0)
\end{align*}
\]  
(15)

Here A, B, C, D, E are undetermined coefficients, σ is the
core charge density on particle surface, \( \mathcal{H}(\theta - \theta_0) \) is Heaviside function, and 2θ0 is the charge distribution angle on
particle surface. The undetermined coefficients can be
determined through the above equations and the boundary
conditions:

\[
\begin{align*}
  & E_c = \frac{3\varepsilon_r \varepsilon_0 (t_2 - t_1) E_0}{(e_2 - e_0) a_1 - (e_1 - e_0) a_2} \\
  & A_1 = -\frac{(e_1 t_1 - e_0 t_1) E_0}{e_2 (t_1 - t_0) a_1} \\
  & A_2 = \frac{-e_2 t_1 - e_1 t_1}{e_2 (t_2 - t_1) a_1} \\
  & A = \frac{-\sigma}{\varepsilon_h} \mathcal{H}(\theta - \theta_0) r_1 \\
  & D = \frac{-\sigma}{\varepsilon_h} \mathcal{H}(\theta - \theta_0) r_1^2
\end{align*}
\]

Here \( a_{1,2} = (e_1 t_1 + e_2 t_2) \), \( x \), \( z = t_1 / r_0 \), and

\[
\begin{align*}
  & e_q = \frac{(e_1 t_2 - e_0 t_1) a_1^2 t_2 - (e_1 t_1 - e_0 t_2) a_1}{(e_1 t_2 - e_0 t_1) a_2^2 t_2 - (e_1 t_1 - e_0 t_2) a_2}
\end{align*}
\]  
(16)

Compared with the results showed in Ref. [35], we can
find that the parameter \( \tilde{\varepsilon}_q \) in the Eq. (16) can be regard as
the equivalent permittivity of the partially charged core-
shell particle with an anisotropic shell. In addition, the
parameter \( \tilde{\varepsilon}_q \) is exactly the same as Eq. (5) in this paper.
Therefore, we can believe that the surface charge on parti-
cle does not change the expression of equivalent per-
mittivity for the inhomogeneous particle or the anisotropic
particle. So we can speculate that, for a spherical particle
with multilayered structure, its equivalent permittivity can
be calculated via Eqs. (5), (6), (9), (11), (12), no matter its
surface is charged or not, even if its shells are anisotropic
medium.

3. Conclusion

This paper, based on the method proposed in the
reference [27], proposed the equivalent permittivity of
layered spherical particle with different forms of coatings
under the Rayleigh hypothesis, and deduced its iteration
relations of the corresponding equivalent permittivity
while those particles have some isotropic coatings, or
some anisotropic coatings, and even them have certain
intervals. In addition, we give the expansion coefficients
of the electric potentials in the core area of particle. Mean-
while, the paper also discussed whether the charges
distributed on the particle surface change the expression of
equivalent permittivity of layered particle or not. However,
those theoretical expressions are just suitable to the con-
tion that the particle size is much smaller than the
wavelength of the incident wave. The study, nevertheless,
can be used to simulate the electrical, optical properties of
layered spheres and those for the functional graded
material in different subjects.

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