METHODOLOGICAL NOTES

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On the problem of the effective parameters of metamaterials

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Contents

__Abstract.__ **The mixing formulas for calculating the effective parameters of composite materials with inclusions having a negative permeability or permittivity are analyzed. The problems appearing when various formulas are utilized were outlined, and the computation algorithms yielding physically meaningful solutions were described. The problem of the calculation of a refractive index for media with arbitrary values of permittivity and permeability is discussed.**

1. Introduction

Metamaterials have recently received much attention in electrodynamics and optics [1 – 10]. The term metamaterials has been born during the study of artificial media to distinguish such media inside which the interaction of electromagnetic waves with inclusions is of substantially nonpotential (retardation) character. Retardation over an inclusion size results in many interesting phenomena, such as chirality [11], artificial magnetism [12 – 18], and so forth. These new properties become most pronounced upon resonance excitation of inclusions.

Beyond these properties, in resonance excitation of inclusions there are frequencies at which the induced electric (magnetic) moment and an applied field oscillate in antiphase that can result in negative values of effective permeability and permittivity. Composites containing highly conducting needles [19] or inclusions with a more complex shape [16, 20 – 23] can serve here as examples. In a restricted sense, by metamaterials are meant media with negative permeability and permittivity. According to this definition, many natural substances can also be attributed to metamaterials; some of them are ferrites and semiconductors at frequencies close to ferromagnetic and exciton resonances, respectively, and many are metals in the IR and optical regions.

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Even if only one of the two characteristics (permeability and permittivity) has a negative value we can encounter many interesting phenomena, namely, the excitation of surface waves and volume Mie resonance modes in individual inclusions [24, 25]. If both permeability and permittivity become negative, this qualitatively changes the optics of such media and allows one to reproduce near-field effects (superresolution, energy transfer by evanescent waves, etc.) on scales comparable to or larger than a wavelength (see Ref. [2]).

In this work, we will not dwell on the physics of all these phenomena and will focus on the mathematical difficulties that appear when media with negative permeability and permittivity are examined. To describe the properties of metamaterials, one has to separate single-valued branches of analytical functions of several complex variables. At present, mathematics yields no unambiguous algorithm to separate such branches. Therefore, researchers use a variety of approaches and statements [26 – 28]. The purpose of this work is to formulate a problem for mathematicians and to provide some recommendations for physicists, which allow them to yield physically sound solutions.

2. Mixing formulas (homogenization theory)

We will first consider a case where the problems discussed above can be reduced to solving well-known problems, namely, the quasistatic case. In the quasistatic approximation, the electric and magnetic problems are known to be solved separately [29]. Actually, this means that we are dealing with single-negative (SNG) media, where either permeability or permittivity takes on negative value, rather than with double-negative (DNG) media, where both permeability and permittivity become negative.

The theory of the effective parameters of composite materials has a long history (see review [30]). It contains both exact results (the so-called two-scale homogenization theory [31, 32], the Dykhne formula [33]) and a whole set of phenomenological theories giving mixing formulas, i.e., formulas that can be used in calculating the effective permeability and permittivity from a given composition of the composite [34 – 57]. The best known mixing formulas are represented by the Garnett [34], von Bruggeman [46], and symmetrized Garnett [53 – 57] formulas. Notice that the two-scale homogenization theory can be rigorously grounded only in the case of problems with a positively defined operator [32]. The extension of the results of this theory to the case of metamaterials has a 'force', i.e., phenomenological, character. From a rigorous theory viewpoint, the application of phenomenological theories, as it usually is, has an uncontrolled character. Moreover, in contrast to a rigorous theory, each of the phenomenological theories qualitatively describes only some properties of a system. [1]

The Bergman – Milton spectral theory should also be noted; negative permittivity (permeability) inclusions play a specific role in this theory. For example, in terms of the Bergman – Milton theory, Bergman [62] showed that the calculation of effective permittivity ε_{eff} can be reduced to finding a spectral function which, in turn, is determined by the distribution of ε_{eff} poles as a function of the permittivities of the inclusions. Although the Bergman – Milton theory does not generate an algorithm to calculate the spectral function, it demonstrates that all effective permittivity poles lie on a negative real axis [62].

Below, we will consider the application of the best known phenomenological theories to describing metamaterials.

In some way or other all phenomenological mixing-formula theories reduce a multiparticle problem to solving a single-particle problem. As a preliminary we analyze the 'perturbation theory' or the 'gas approximation' — that is, the case where the inclusion concentration is so low that we may neglect the effect of particles on each other.

Following Ref. [29], we write out the integral

$$\mathbf{I} = \frac{1}{V}\int (\mathbf{D} - \varepsilon_{\text{m}}\mathbf{E})\,\mathrm{d}v = \langle \mathbf{D} \rangle - \varepsilon_{\text{m}}\langle \mathbf{E} \rangle\,, \tag{1}$$

where ε_{m} and ε_{i} are the permittivities of the matrix and inclusion, respectively. Effective permittivity ε_{eff} is determined from the equation $\langle \mathbf{D} \rangle = \varepsilon_{\text{eff}}\langle \mathbf{E} \rangle$ and can be expressed through the integral $\mathbf{I}$:

$$\langle \mathbf{D} \rangle = \varepsilon_{\text{eff}}\langle \mathbf{E} \rangle = \varepsilon_{\text{m}}\langle \mathbf{E} \rangle + \mathbf{I}\,. \tag{2}$$

Taking into account that the integrand is nonzero only inside an inclusion, where $\mathbf{D} = \varepsilon_{\text{i}}\mathbf{E}$, for integral $\mathbf{I}$ we obtain

$$\mathbf{I} = \frac{1}{V}\int (\mathbf{D} - \varepsilon_{\text{m}}\mathbf{E})\,\mathrm{d}v = \frac{1}{V}\int (\varepsilon_{\text{i}} - \varepsilon_{\text{m}})\mathbf{E}\,\mathrm{d}v\,, \tag{3}$$

where the last integral is taken over the volume of the inclusions.

We neglect the spatial change in the so-called local field $\mathbf{E}_{\text{loc}}$, in which the inclusion is located, and obtain the well-known expression [29]

$$\mathbf{E}_{\text{i}} = \frac{3\varepsilon_{\text{m}}}{\varepsilon_{\text{i}} + 2\varepsilon_{\text{m}}}\,\mathbf{E}_{\text{loc}} \tag{4}$$

for the field inside the inclusion, which yields the equation

$$\langle \mathbf{D} \rangle = \varepsilon_{\text{m}}\langle \mathbf{E} \rangle + p\,\frac{3\varepsilon_{\text{m}}(\varepsilon_{\text{i}} - \varepsilon_{\text{m}})}{\varepsilon_{\text{i}} + 2\varepsilon_{\text{m}}}\,\mathbf{E}_{\text{loc}}\,, \tag{5}$$

where p is the inclusion volume concentration.

[1] Here, we do not consider the problem of the validity of introducing the effective permeability and permittivity for composites in circumstances where the resonance interaction of electromagnetic waves with inhomogeneities occurs. We refer the reader to works [23, 58 – 61] where this problem is discussed.

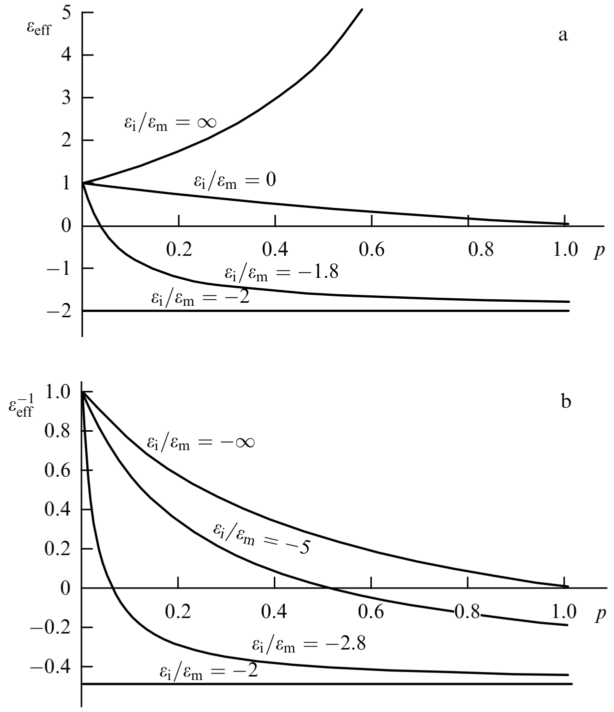

Figure 1. Effect of concentration p on (a) ε_{eff} and (b) $\varepsilon_{\text{eff}}^{-1}$ at various values of $\varepsilon_{\text{i}}/\varepsilon_{\text{m}}$. The curves were constructed using the Garnett formula (8).

To this point, we have only assumed that particles are located in a uniform external field and that the interparticle distance is much larger than the particle size, so that we may neglect the changes in the fields of other particles on the scale of any individual inclusion.

We then assume that the fields of other particles are neglected (gas approximation), i.e., $\mathbf{E}_{\text{loc}} = \mathbf{E}_{\text{ext}}$, and obtain the following expression for calculating the effective permittivity:

$$\varepsilon_{\text{eff}} = \varepsilon_{\text{m}} + p\,\frac{3\varepsilon_{\text{m}}(\varepsilon_{\text{i}} - \varepsilon_{\text{m}})}{\varepsilon_{\text{i}} + 2\varepsilon_{\text{m}}}\,. \tag{6}$$

If we calculate the local field using the Lorentz – Lorenz formula [36 – 39]

$$\mathbf{E}_{\text{loc}} = \langle \mathbf{E} \rangle + \frac{4\pi}{3}\,\mathbf{P}\,, \tag{7}$$

where $\langle \mathbf{E} \rangle$ is the mean field, $\mathbf{E}_{\text{loc}}$ is the local field, and $\mathbf{P}$ is the particle polarization, we derive the well-known Garnett formula

$$\varepsilon_{\text{eff}} = \varepsilon_{\text{m}} + 3p\,\frac{\varepsilon_{\text{m}}(\varepsilon_{\text{i}} - \varepsilon_{\text{m}})}{(\varepsilon_{\text{i}} + 2\varepsilon_{\text{m}}) - p(\varepsilon_{\text{i}} - \varepsilon_{\text{m}})}\,, \tag{8}$$

where ε_{m} and ε_{i} are the permittivities of the matrix and inclusion, respectively, and p is the inclusion volume concentration. This formula is notable, since it takes into account real boundary conditions, which is extremely important in the presence of volume and surface modes [63].

As applied to negative permittivity inclusions, Eqns (6) and (8) bring up no mathematical problems. Figure 1 depicts the concentration dependences of ε_{eff}.

Until $\varepsilon_{\text{i}} > -2\varepsilon_{\text{m}}$, ε_{eff} changes monotonically from ε_{m} to ε_{i} as the inclusion concentration increases from zero to unity

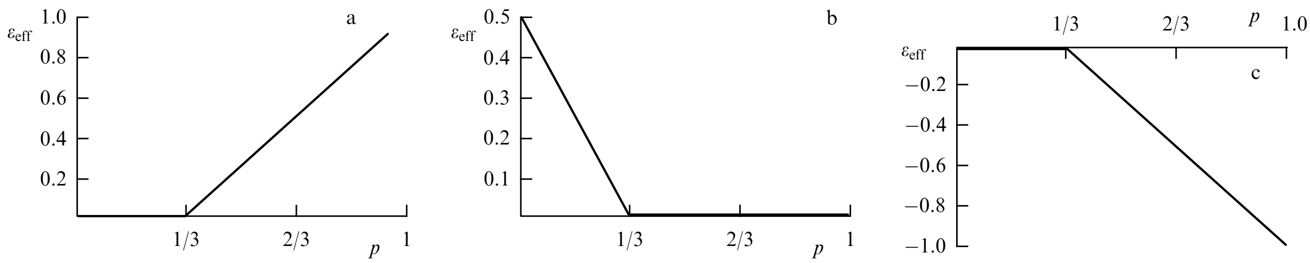

Figure 2. Dependences of the effective permittivity on concentration p that illustrate a percolation transition as $\varepsilon_{\mathrm{m}}/\varepsilon_{\mathrm{i}} \to 0$ in accordance with the EMT: (a) $\varepsilon_{\mathrm{i}} = 1$, (b) incorrect result (13) at $\varepsilon_{\mathrm{i}} = -1$, and (c) correct result obtained from Eqn (14) at $\varepsilon_{\mathrm{i}} = -1$.

(Fig. 1a).[2] For negative permittivity inclusions there is a concentration at which the effective permittivity vanishes, which is in complete agreement with the Bergman–Milton spectral theory. For $\varepsilon_{\mathrm{i}} < -2\varepsilon_{\mathrm{m}}$, it is more convenient to analyze the function $\varepsilon_{\mathrm{eff}}^{-1}$, because a permittivity pole other than zero appears — that is, the effective permittivity becomes infinite, which is related to an 'electromagnetic trap' phenomenon at $\varepsilon_{\mathrm{i}} = -2\varepsilon_{\mathrm{m}}$. To meet this condition, the dipole moment of the inclusion and the local field along with it become infinite, which gave the name to this phenomenon. When delay effects are taken into account, the field and dipole moment become restricted, which follows from the rigorous Mie theory [23, 24].

When the condition $\varepsilon_{\mathrm{i}} = -2\varepsilon_{\mathrm{m}}$ is exactly satisfied, the effective permittivity ceases to depend on the concentration (the pole is located at $p = 0$): $\varepsilon_{\mathrm{eff}} = -2\varepsilon_{\mathrm{m}}$. When ε_{i} tends to minus infinity, the pole moves toward unity (see Fig. 4, dashed line). Given permittivity and permeability, $\varepsilon_{\mathrm{eff}}^{-1}$ changes monotonically from $\varepsilon_{\mathrm{m}}^{-1}$ to $\varepsilon_{\mathrm{i}}^{-1}$ (Fig. 1b).

In the von Bruggeman theory, which is often called the effective medium theory (EMT), a matrix and inclusions are considered to be equivalent. This formula is often called a symmetric mixing formula. The EMT assumes that, on average, particles do not disturb an external field — that is, on average, the field inside the particles is equal to the applied field. In this case, particles consisting of the inclusion material and those consisting of the matrix material are considered to be embedded in a certain homogeneous medium with the desired permittivity $\varepsilon_{\mathrm{eff}}$. An equation for finding $\varepsilon_{\mathrm{eff}}$ takes the form

$$\sum_i p_i \mathbf{E}_{\mathrm{int}}^{(i)} = \mathbf{E}_0 \,,$$

where summation is taken over all types of materials.

With Eqn (4), we can rewrite this equation for a two-component mixture in the form

$$p\,\frac{\varepsilon_{\mathrm{eff}} - \varepsilon_{\mathrm{i}}}{2\varepsilon_{\mathrm{eff}} + \varepsilon_{\mathrm{i}}} + (1-p)\,\frac{\varepsilon_{\mathrm{eff}} - \varepsilon_{\mathrm{m}}}{2\varepsilon_{\mathrm{eff}} + \varepsilon_{\mathrm{m}}} = 0 \,. \tag{9}$$

The EMT has many modifications which try to take into account specific phenomena or properties of composites that are not described by the von Bruggeman formula. For example, the authors of Refs [22, 64] obtained an expression that takes into account the skin effect in metallic inclusions, and the formula proposed in Ref. [47] includes a percolation threshold as a free parameter. In Refs [23, 65, 66], researchers tried to take into account correlations in a particle distribution. All these approaches are based on Eqn (9).

The popular appeal of Eqn (9) is based on the fact that it describes a percolation transition at $p_{\mathrm{c}} = 1/3$ (in the Garnett theory, the percolation threshold is equal to unity). In other words, at $\varepsilon_{\mathrm{m}} = 0$, the effective permittivity $\varepsilon_{\mathrm{eff}}$ is identically zero at concentrations below a percolation threshold and changes from zero to ε_{i} as the inclusion concentration increases from the percolation threshold to unity. However, even to obtain this result, one has to carefully manipulate the functions of a complex variable.

Indeed, when ε_{m} tends to zero, the second term in Eqn (9) has the form of an uncertainty of the $0/0$ type, and to obtain the right answer, we have to utilize the general solution to Eqn (9) in the form

$$\varepsilon_{\mathrm{eff}} = 0.25\Big[\varepsilon_{\mathrm{i}}(3p-1) + \varepsilon_{\mathrm{m}}(2-3p) + \sqrt{\big[\varepsilon_{\mathrm{i}}(3p-1) + \varepsilon_{\mathrm{m}}(2-3p)\big]^2 + 8\varepsilon_{\mathrm{i}}\varepsilon_{\mathrm{m}}}\,\Big] \,. \tag{10}$$

Here, we encounter the problem of choosing a single-valued analytical branch of the root for the first time. The physically right answer (passive inclusions give a passive effective medium, and active inclusions give an active effective medium) generates a cut along the negative real axis and defines the square root as follows

$$\sqrt{z} = \sqrt{|z|}\,\exp\left(\mathrm{i}\,\frac{1}{2}\,\varphi_z\right) \quad \text{for} \quad -\pi < \varphi_z < \pi \,. \tag{11}$$

Then, in the limit $\varepsilon_{\mathrm{m}} \to 0$ and $\varepsilon_{\mathrm{i}} > 0$, the EMT yields the percolation behavior (Fig. 2a):

$$\varepsilon_{\mathrm{eff}} = 0.25\Big[\varepsilon_{\mathrm{i}}(3p-1) + \sqrt{\big[\varepsilon_{\mathrm{i}}(3p-1)\big]^2}\,\Big] = 0.25\Big[\varepsilon_{\mathrm{i}}(3p-1) + \big|\varepsilon_{\mathrm{i}}(3p-1)\big|\Big] = \begin{cases} 0\,, & p < p_{\mathrm{c}}\,, \\ \dfrac{\varepsilon_{\mathrm{i}}(3p-1)}{2}\,, & p > p_{\mathrm{c}}\,. \end{cases} \tag{12}$$

However, to obtain analogous behavior for $\varepsilon_{\mathrm{i}} < 0$, we should choose another branch of the square root; otherwise, the strange result

$$\varepsilon_{\mathrm{eff}} = \begin{cases} \dfrac{\varepsilon_{\mathrm{i}}(3p-1)}{2}\,, & p < p_{\mathrm{c}}\,, \\ 0\,, & p > p_{\mathrm{c}} \end{cases} \tag{13}$$

is obtained (Fig. 2b), which robs this approach of universality. This is caused by the fact that we are dealing with a

[2] Note again that these formulas were derived in the low-concentration approximation, where the interparticle distance is much larger than the particle size. Researchers often forget this assumption and apply these formulas at high concentrations, which can lead to physically unreasonable results.

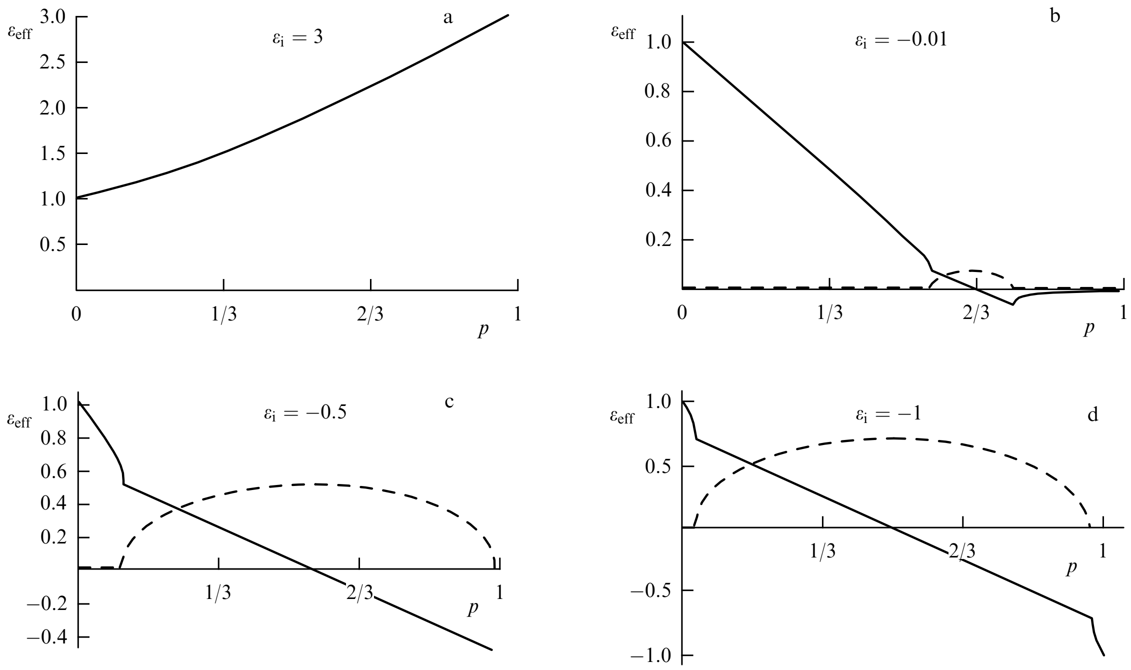

Figure 3. Dependences of $\mathrm{Re}\,\varepsilon_{\rm eff}$ (solid line) and $\mathrm{Im}\,\varepsilon_{\rm eff}$ (dashed line) on the volume fraction p of inclusions according to the EMT at $\varepsilon_{\rm m} = 1$ and various values of the parameter $\varepsilon_{\rm i}$.

function of many complex variables. The problem of separating a single-valued analytical branch of a function of several complex variables still has no final solution [67, 68]. It seems reasonable to reduce the problem to the calculation of the functions of one variable by factorizing the argument $\sqrt{z_1 \times \ldots \times z_n} = \sqrt{z_1} \times \ldots \times \sqrt{z_n}$ [67, 68]. As a result, we obtain the expression

$$\varepsilon_{\rm eff} = 0.25\left[\varepsilon_{\rm i}(3p-1) + \sqrt{\varepsilon_{\rm i}}\,\sqrt{\varepsilon_{\rm i}}\,\sqrt{(3p-1)^2}\,\right] \qquad (14)$$

instead of formula (12), which furnishes the right percolation behavior (Fig. 2c). It should be noted that we employed the expression

$$\sqrt{\varepsilon_{\rm i}^2} = \sqrt{\varepsilon_{\rm i}}\,\sqrt{\varepsilon_{\rm i}} = \varepsilon_{\rm i}$$

in order to extract the root of the permittivity squared, and we applied the traditional formula

$$\sqrt{(3p-1)^2} = |3p-1|$$

from the theory of functions of a real variable in order to extract the root of the remaining expression.

To find the solution in the general case of $\varepsilon_{\rm m} \neq 0$, we propose using an expression of the type

$$\varepsilon_{\rm eff} = 0.25\Bigg[\varepsilon_{\rm i}(3p-1) + \varepsilon_{\rm m}(2-3p) + \sqrt{\varepsilon_{\rm i} - \varepsilon_{\rm m}\,\frac{9p^2 - 9p - 2 + 6\sqrt{2p(1-p)}}{(1-3p)^2}} \times \sqrt{\varepsilon_{\rm i} - \varepsilon_{\rm m}\,\frac{9p^2 - 9p - 2 - 6\sqrt{2p(1-p)}}{(1-3p)^2}}\,\sqrt{(3p-1)^2}\,\Bigg]\,. \qquad (15)$$

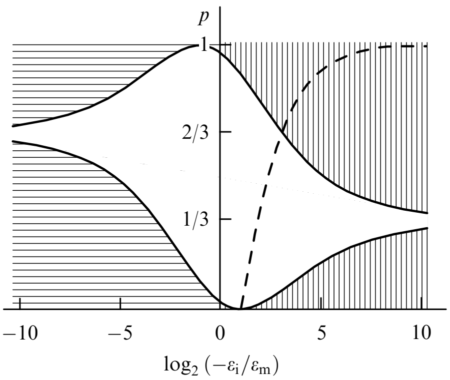

Figure 4. Characteristic points of the $\varepsilon_{\rm eff}(p)$ curve depending on the $\varepsilon_{\rm i}/\varepsilon_{\rm m}$ ratio. The unhatched region corresponds to the complex values of $\varepsilon_{\rm eff}$ obtained from the EMT; the horizontal hatching corresponds to the region where the $\varepsilon_{\rm eff}(p)$ function is convex up $(\mathrm{d}^2\varepsilon_{\rm eff}/\mathrm{d}p^2 < 0)$, while the vertical hatching corresponds to the region where this function is convex down. In the unhatched region, one has $\mathrm{Re}\,(\mathrm{d}^2\varepsilon_{\rm eff}/\mathrm{d}p^2) = 0$. The dashed line illustrates the position of the pole according to the Garnett formula.

The results of calculations utilizing this formula are given in Fig. 3. The absence of poles is a specific feature, which is related to breaking the plasmon resonance condition (effective rather than real boundary conditions are considered) and to the presence of a concentration region where the effective permittivity has an imaginary part (Fig. 4). The appearance of 'dissipation' is associated with energy 'pumping' into the forming resonance configurations [33].

The symmetrized Garnett formula [53 – 57] generates both a percolation transition and resonance behavior. In this approach, one considers the probability $P_{\rm I}$ of those configurations where an inclusion is surrounded by matrix material, and the probability $P_{\rm II}$ of configurations where a matrix particle is surrounded by an inclusion material. As was shown

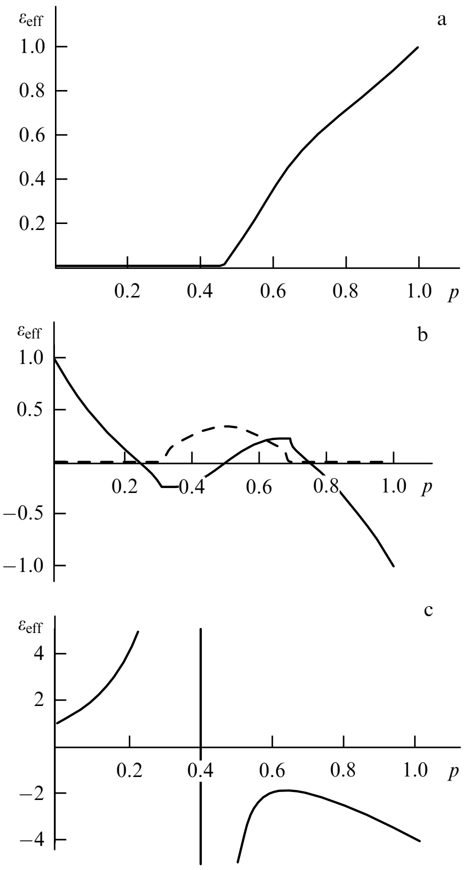

Figure 5. Dependences of Re ε_{eff} (solid line) and Im ε_{eff} (dashed line) on the volume fraction p of inclusions according to the symmetrized Garnett formula at the following values of the parameters: (a) $\varepsilon_{\text{m}} \to 0$, $\varepsilon_{\text{i}} = 1$; (b) $\varepsilon_{\text{m}} = 1$, $\varepsilon_{\text{i}} = -1$, and (c) $\varepsilon_{\text{m}} = 1$, $\varepsilon_{\text{i}} = -4$.

in Ref. [53], the appropriate probabilities are given by

$$P_{\text{I}} = \frac{u_{\text{I}}}{u_{\text{I}} + u_{\text{II}}}\,, \qquad P_{\text{II}} = \frac{u_{\text{II}}}{u_{\text{I}} + u_{\text{II}}}\,,$$

where

$$u_{\text{I}} = (1 - p^{1/3})^3\,, \qquad u_{\text{II}} = \left[1 - (1-p)^{1/3}\right]^3\,.$$

For each of the configurations I and II, we calculate the effective permittivity using the Garnett theory,

$$\varepsilon_{\text{I}} = \varepsilon_{\text{m}} + 3p\,\frac{\varepsilon_{\text{m}}(\varepsilon_{\text{i}} - \varepsilon_{\text{m}})}{(\varepsilon_{\text{i}} + 2\varepsilon_{\text{m}}) - p(\varepsilon_{\text{i}} - \varepsilon_{\text{m}})}\,,$$

$$\varepsilon_{\text{II}} = \varepsilon_{\text{i}} + 3(1-p)\,\frac{\varepsilon_{\text{i}}(\varepsilon_{\text{m}} - \varepsilon_{\text{i}})}{(\varepsilon_{\text{m}} + 2\varepsilon_{\text{i}}) - (1-p)(\varepsilon_{\text{m}} - \varepsilon_{\text{i}})}\,,$$

which correctly describe possible resonances. At the second step, we perform averaging over the configurations in terms of the EMT. Since other configurations are assumed to be absent, the equation for the effective permittivity has the form

$$P_{\text{I}}\,\frac{\varepsilon_{\text{eff}} - \varepsilon_{\text{I}}}{2\varepsilon_{\text{eff}} + \varepsilon_{\text{I}}} + P_{\text{II}}\,\frac{\varepsilon_{\text{eff}} - \varepsilon_{\text{II}}}{2\varepsilon_{\text{eff}} + \varepsilon_{\text{II}}} = 0\,.$$

This theory gives a finite percolation threshold $p_{\text{c}} \approx 0.455$ (Fig. 5a). On the whole, the behavior of the effective

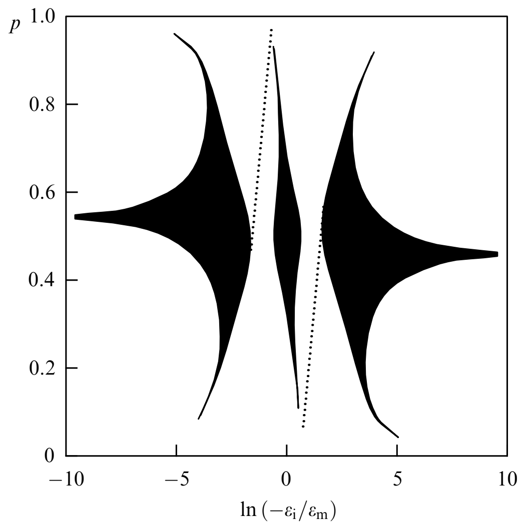

Figure 6. Behavior of the ε_{eff} function calculated using the symmetrized Garnett formula. The shaded regions correspond to complex values of ε_{eff}. The dotted lines indicate the position of the pole.

permittivity has a rather complex character: there are regions with bands and effective dissipation (Fig. 5b, c, and Fig. 6).

3. Choice of the refractive index sign for the Veselago medium

Unfortunately, the approach developed above cannot always be extended to other problems, e.g., to the refractive index calculation. Specifically, we cannot factorize the argument to restrict ourselves to only one analytical branch. This is related to the fact that we should determine both the refractive index and impedance. In the case where both permittivity and permeability are passive ($\varepsilon'' > 0$, $\mu'' > 0$) or active ($\varepsilon'' < 0$, $\mu'' < 0$), we can utilize the factorization algorithm $\sqrt{z_1 z_2} = \sqrt{z_1}\,\sqrt{z_2}$ described above and can determine the refractive index using the formula $n = \sqrt{\varepsilon}\,\sqrt{\mu}$ [58]. One can readily see that, when losses for the Veselago medium are neglected ($\varepsilon' < 0$, $\mu' < 0$), the refractive index becomes negative. However, in a mixed case, for example, when the medium is electrically active and magnetically passive, we have to take another branch of the root, which makes it necessary to search for a more reliable and unambiguous algorithm for finding the refractive index.

Against the background of these difficulties, researchers discuss the method and validity of the introduction of a negative refractive index (see Ref. [26]). The authors of Refs [26, 28] believe that the refractive index and impedance describe the properties of a wave propagating in the medium rather than the properties of the medium, and that researchers should operate with permittivity and permeability rather than with these variables. Although this approach makes some sense, we will inevitably come to the problem of the calculation of square roots for practical purposes (solution of integral equations in diffraction problems, waveguide system calculation, etc.).

Note that the conventional Maxwell equations with permeability and permittivity, viz.

$$\begin{aligned} [\mathbf{k} \times \mathbf{E}] &= k_0 \mu \mathbf{H}\,, \\ [\mathbf{k} \times \mathbf{H}] &= -k_0 \varepsilon \mathbf{E}\,, \end{aligned} \tag{16}$$

where $k_0 = \omega/c$, can be rewritten using the refractive index $n = \sqrt{\varepsilon\mu}$ and impedance $\zeta = \sqrt{\mu/\varepsilon}$:

$$[\mathbf{k} \times \mathbf{E}] = (k_0 n)(\zeta \mathbf{H}),\qquad \big[\mathbf{k} \times (\zeta \mathbf{H})\big] = -(k_0 n)\mathbf{E}. \tag{17}$$

Although this approach has many disadvantages (especially when moving to statics), it turns out to be useful in our case. It is seen from the relations

$$\mu = n\zeta, \qquad \varepsilon = \frac{n}{\zeta} \tag{18}$$

that the signs of n and ζ for the Veselago medium should be different; whence it follows that the propagating wave is a backward wave. Indeed, the Poynting vector in the absence of losses is expressed through a wavevector, refractive index, and impedance as follows:

$$\mathbf{S} = \frac{c}{8\pi}\,\mathrm{Re}\,[\mathbf{E} \times \mathbf{H}^*] = \frac{c}{8\pi}\,\frac{\mathbf{k}}{k_0}(\mathbf{E}\mathbf{E}^*)\,\frac{1}{\zeta n}. \tag{19}$$

For media with a negative permittivity and permeability, we have $\zeta n = \mu < 0$. As a consequence, the Poynting vector and the wavevector are oppositely directed.

It should be noted that the sign of the refractive index is still undetermined, and we face the following two variants (in complete accordance with the conclusions of Ref. [26]):

$$\zeta > 0, \qquad n < 0, \tag{20a}$$

$$\zeta < 0, \qquad n > 0. \tag{20b}$$

In addition, the authors of Ref. [26] stated that this dilemma is likely to be insolvable in terms of the Maxwell equations. The formal use of the dispersion equation

$$k^2 = (k_0 n)^2 \Rightarrow k = \pm k_0 \sqrt{\varepsilon\mu} \tag{21}$$

needs additional information for choosing the analytical branch required at a certain time.

In Ref. [26], both n and k (wavevector magnitude) were assumed to be positive, and the sign ambiguity is then transferred to the choice of the direction of the unit vector: $\mathbf{k} = k\boldsymbol{\tau}$. If the refractive index is taken to have a positive sign, we should direct $\boldsymbol{\tau}$ oppositely to the Poynting vector and change the sign in the formulas that describe the phenomena depending only on the refractive index in the case of the Veselago medium. For example, the Snell law takes the form

$$\frac{\sin\vartheta}{\sin\vartheta'} = -n, \tag{22}$$

where ϑ is the angle of incidence in a vacuum, and ϑ' is the angle of refraction. This is rather inconvenient, since we have to know the type of medium *a priori* in order to write out a certain formula. Moreover, this does not save the situation, because the question of choosing the $\boldsymbol{\tau}$ direction is still open.

It is more convenient and, apparently, correct to fix the sign of the real part of impedance rather than the sign of the refractive index, as was done in Ref. [26]. In addition, it is generally accepted that the real part of impedance is chosen to be positive [29], which leads to version (20a) in the case of the Veselago medium, and to the standard expression for the refractive index in the case of ordinary media. As in the case of work [26], this unambiguously determines the sign of the refractive index, and the only difference consists in the fact that all the formulas (the Snell law, the Doppler effect, etc.) have the same form for all cases. Any branch of the square root can be used here, but the same branch should be used when calculating n and ζ. If the sign of $\mathrm{Re}\,\zeta$ proved to be negative, this means that we are dealing with a wave propagating in the opposite direction.

To support the correctness of this approach, we address work [69], where the following expression for the electromagnetic energy density in a dispersive medium was rederived in an original manner:

$$\begin{aligned} w &= \frac{1}{16\pi}\left\{\frac{\mathrm{d}(\omega\varepsilon)}{\mathrm{d}\omega}\,EE^* + \frac{\mathrm{d}(\omega\mu)}{\mathrm{d}\omega}\,HH^*\right\} \\ &= \frac{1}{16\pi}\left\{\frac{\mathrm{d}(\omega\varepsilon)}{\mathrm{d}\omega} + \frac{\mu}{\varepsilon}\,\frac{\mathrm{d}(\omega\mu)}{\mathrm{d}\omega}\right\}EE^* \\ &= \frac{c}{8\pi}\sqrt{\frac{\varepsilon}{\mu}}\,\frac{\mathrm{d}k}{\mathrm{d}\omega}\,EE^* = \frac{c}{8\pi}\,\frac{1}{\zeta v_{\mathrm{gr}}}\,EE^*. \end{aligned} \tag{23}$$

It is natural to assume that the energy density is positive. Following Sivukhin [69] (see also Ref. [29]), we write out Eqn (23) in the form

$$\begin{aligned} w &= \frac{\mu}{\mu}\,\frac{c}{8\pi}\sqrt{\frac{\varepsilon}{\mu}}\,\frac{\mathrm{d}k}{\mathrm{d}\omega}\,EE^* = \frac{c}{8\pi}\,EE^*\left(\mu\,\frac{1}{\sqrt{\varepsilon\mu}}\,\frac{\mathrm{d}\omega}{\mathrm{d}k}\right)^{-1} \\ &= \frac{1}{8\pi}\,EE^*\left(\mu\,\frac{\omega}{k}\,\frac{\mathrm{d}\omega}{\mathrm{d}k}\right)^{-1} > 0. \end{aligned} \tag{24}$$

"This inequality should hold true for any media in which the signs of ε and μ coincide, since it was derived on the assumption that a homogeneous monochromatic wave, for which

$$k^2 = \frac{\omega^2}{c^2}\,\varepsilon\mu > 0,$$

can propagate in a medium. With the same assumption, we can also speak about group and phase velocities...; as a result, the following inequality can readily be obtained:

$$\mu\,\frac{\omega}{k}\,\frac{\mathrm{d}\omega}{\mathrm{d}k} = \mu v_{\mathrm{ph}} v_{\mathrm{gr}} > 0.\text{" [69]} \tag{25}$$

Thus, at negative values of ε and μ, the signs of the group and phase velocities are different. Recall that a group velocity is related to energy and information transfer [70, 71]. Therefore, it is precisely this quantity that should be considered as a positive quantity [28]. We return to expression (23) and find that impedance should be positive. Indeed, formulas (23) and (24) yield $\zeta v_{\mathrm{gr}} > 0$.

The final algorithm for the determination of the refractive index consists in the choice of the single-valued branch of the square root that gives a positive real part of the characteristic impedance. The position of the cut that specifies two single-valued analytical branches of the square root is of no importance here. The branch with a negative real part of the impedance corresponds to a wave moving in the negative direction — that is, the minus sign should be used in expression (21). Finally, the dispersion relation takes the form

$$k = \mathrm{sgn}\,(\mathrm{Re}\,\zeta)\,k_0 n. \tag{26}$$

Thus, to determine the sign of the refractive index and the right sign in the dispersion relation, we should consider the wave with which these notions are related (see also Ref. [28]). Using relation (26) and one of the pairs in Eqn (20), we will correctly describe the wave propagation.

Although we have analyzed nondissipative media, algorithm (26) gives the right sign of the refractive index in the general case, in particular, in the case where the permittivity of the medium is passive and its permeability is active, or vice versa.

4. Conclusion

When calculating the material parameters of metamaterials, researchers encounter the problem of choosing a single-valued analytical branch of a function of several complex variables. Although a developed mathematical theory is absent, we used a quasistatic approximation and constructed an algorithm that gives an unambiguous, physically correct solution to finding the effective permittivity and permeability of composite materials with a negative permittivity or permeability. However, the solution to the problem of choosing a single-valued branch that appears when electrodynamic phenomena are described using the refractive index – impedance pair rather than the permittivity – permeability pair requires additional physical concepts, namely, the requirement of a positive real part of impedance. The necessity of using different branches of an analytical function appears when researchers analyze media that are simultaneously magnetically passive (the imaginary part of the permeability is positive) and electrically active (the imaginary part of the permittivity is negative), or vice versa. It should be noted that in all other cases, including the case of positive permittivity and permeability, we can define the refractive index as $n = \sqrt{\varepsilon}\,\sqrt{\mu}$ and restrict ourselves to only one branch of the square root with a cut running along the negative real axis.

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