Extinction coefficient in absorbing media: a theoretical and numerical study

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Abstract

We report a theoretical and numerical investigation of the light scattering in an absorbing medium with randomly distributed scatterers. The extinction coefficient is derived from the imaginary part of the effective index derived using a diagrammatic approach. The accuracy of the result is assessed by comparison with a numerical solution of Maxwell's equations that fully accounts for multiple scattering.

1 Introduction

Modelling transport of light in scattering random media when the host medium is absorbing is a fundamental topic of practical importance. In this paper, we focus on the extinction coefficient in absorbing media containing a random distribution of scatterers of arbitrary size. No general satisfying form of the extinction coefficient has been derived yet. Indeed, the presence of the particles modifies the field in the host medium. Hence the absorption in the host medium is also modified by the presence of particles. In other words, particles and host medium cannot be treated as two uncoupled systems. This entails that the scattering and absorption cross-section are not intrinsic characteristics of the particle when the latter is embedded into an absorbing medium. This issue has already been raised by Bohren *et al.*[3] and more recently by Videen *et al.*[2].

The purpose of this paper is to introduce a new model of the extinction coefficient in absorbing media based on the effective medium theory (EMT) arising from the well developed multiple scattering theory[4, 5, 6]. The second section outlines the key ideas of our model. In order to assess the validity of the model, we have implemented a numerical solution of Maxwell equations for a set of 2D particles (cylinders) embedded in an absorbing host medium. We solve the problem for a large number of realizations and perform an ensemble average over typically 500 realizations. Section 3 is devoted to the outline of this procedure. Section 4 shows an example of comparison between numerical simulations and theory.

2 Diagrammatic expansion of the extinction coefficient

The key of our approach is to derive an equation for the mean field in a random medium. This equation has the form of a Helmholtz equation with an effective refractive index. As this effective refractive index is homogeneous, the energy flux due to the mean field coincides with the contribution of the collimated part of the specific intensity. The extinction coefficient K_{ext} is simply related to the imaginary part of the effective wavevector $Im(k_{eff})$:

$$K_{ext} = 2Im(k_{eff}). \tag{1}$$

Within the independent scattering approximation, we show[1] that the effective wave vector is given by:

$$k^2 = k_h^2 + i\frac{f}{v_p}\frac{4\pi S_{k_h}(0)}{k_h}, \tag{2}$$

where $S_{k_h}(0)$ is the scattering matrix as defined by Bohren and Huffman [7] evaluated in the forward direction, v_p is the volume of a particle, f is the filling ratio of particles and the wavevector in the matrix is $k_h = n_h k_0$ where n_h is the host medium refractive index and k_0 is the wavenumber in free space. The effective medium theory can be improved by taking into account the correlation between two particles[6, 1]. It yields the following equation for the effective wavevector:

$$\begin{aligned} k^2 &= k_h^2 + i\frac{f}{v_p}\frac{4\pi S_{k_h}(0)}{k_h} \\ &+ \left(i\frac{f}{v_p}\frac{4\pi S_{k_h}(0)}{k_h}\right)^2 \frac{1}{k}\int_0^\infty e^{ik_h r}\sin(kr)g_2(r)dr, \end{aligned} \tag{3}$$

where $g_2(r)$ is the pair-correlation function[5, 1]. This expression is strictly rigorous only for small particles and assuming a scalar behavior of the corrective terms due to the correlations[1]. We note that this equation can be cast in the form:

$$k^2 = k_0^2 n_{eff}^2(\omega, k), \tag{4}$$

where n_{eff} is an effective index that depends on ω so that the medium is dispersive and on k so that the medium is non-local. In what follows, we will refer to this model as a non-local effective medium. The non-local correction has to be taken into account when correlations cannot be ignored, this is the so-called dependent scattering regime. For the sake of comparison, we report the phenomenological expression introduced by Kuga *et al.*[8] :

$$K_{ext} = 2k_0 Im(n_h)(1-f) + \frac{f}{v_p}C_{ext}, \tag{5}$$

where C_{ext} is the extinction cross section of a scatterer evaluated as if the host medium was not absorbing. This model is based on the simple idea that absorption is a local phenomenon and that the field is essentially uniform. Within this approximation, absorption in the host medium is proportional to the host volume. There are many cases where this approximation is very good. Yet, it is clear that if the particle has a resonance, the field at the boundary is enhanced. In turn, this produces a strong field in the host medium along the boundary. It follows that the presence of the particle may increase the absorption in the host medium. This discussion suggests that it is necessary to account for the exact scattering operator of the particle including the losses of the host medium. In order to compare the 2D numerical simulation with the effective medium theory, we have developped a 2D version of the effective medium theory[1].

3 Derivation of the extinction coefficient from a numerical simulation

We outline in this section the derivation of the extinction coefficient from the exact numerical solution of Maxwell's equation in a slab with a thickness e containing a 2D random distribution of dielectric disks. The host medium is absorbing. We consider a p-polarized incident plane wave. The geometry described in Fig.1 is periodic along the slab with a period L large compared to the wavelength and the particle size in order to avoid edge effects. The periodic system diffracts the incident plane wave into a large number of discrete directions given by the transverse wave number $k_{x,p} = k_{inc,x} + p\frac{2\pi}{L}$, where p is the diffraction order. Disk particles are randomly distributed in the slab with the condition that particles cannot overlap and that each disk is entirely in the rectangular box. For each realization of a random distribution of particles, the reflected and transmitted field is computed exactly using the method of moment as it was described in ref.[9]. Since the scatterers are randomly located, each realization produces a speckle pattern. When considering the set of solutions corresponding to a set of realizations, it proves useful to split the field as the sum of the statistical average and a fluctuating component:

$$\mathbf{E} = <\mathbf{E}> + \delta\mathbf{E}, \tag{6}$$

where $<\delta\mathbf{E}> = 0$. Between 200 and 1000 realizations were generated to compute the average field. When averaging the intensity, the speckle pattern is smoothed and one finds the scattered intensity pattern. When averaging the field, the speckle structure disappears and the mean field is the response of the average system with the effective index. For a slab, we find two plane waves specularly transmitted or reflected.

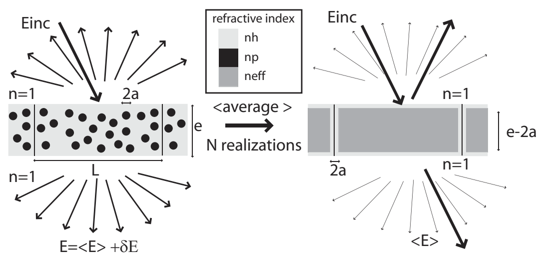

Figure 1: Geometry of the system

4 Comparison between numerical simulations and approximate theories

We have investigated the extinction coefficient in an absorbing medium when the correlation effects are important. Results are displayed in Fig.2 for different cases. We shall discuss the effect of dielectric contrast, losses in the particles and correlation between particles. Our main conclusions can be summarized

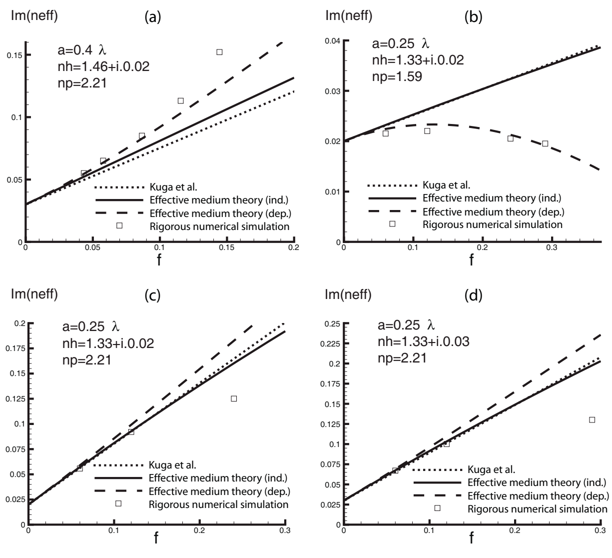

Figure 2: Comparison between theory and numerical simulation

as follows. The comparison shows a very good agreement in the independent scattering regime. When the dielectric contrast between particles and the host medium is small, the EMT model which takes into account the correlation between pair of scatterers is in excellent agreement with the exact result up to 30% as seen in Fig.2. For a filling ratio above 5%, we find that for small particles, the effect of correlations leads to a smaller extinction coefficient than predicted by the independent scattering approximation, while the tendency is reversed for large particles. It is worth noticing that there is a particle size for which the correlation effects are negligible up to 15 $\%$. It is also observed that in general, the absorption of the host medium reduces the effect of the correlations allowing one to use the independent scattering approximation for larger filling ratio. The case of large dielectric contrast, large volume fraction and size parameter on the order of one (the so-called resonance regime) remains an open issue.

5 Conclusion

The evaluation of the extinction coefficient for particles embedded in an absorbing medium is a long standing problem. Using the multiple scattering theory in random media, we have derived the expression of the extinction coefficient from the imaginary part of the effective index for two-dimensional and three-dimensional cases. Taking into account correlation between particles position yields a non-local effective index. In order to assess the accuracy of the model, we have presented in this paper a direct comparison with two-dimensional exact solution of Maxwell's equations in an absorbing slab filled with randomly distributed scatterers.

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