Effect of short-range order on the mean field of a wave in a randomly nonuniform medium

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The Helmholtz equation is solved in the pairwise interaction approximation (also called the Bourret approximation) for the mean field—for an ensemble of realizations—in an unbounded nonuniform medium described by a normalized binary correlation function $\varphi(\mathbf{r}_1,\mathbf{r}_2)=[\exp(-r/a)]\cos(\mathbf{pr})$, where $\mathbf{r}\equiv\mathbf{r}_1-\mathbf{r}_2$, a is the spatial scale of the correlations, and $\mathbf{p}$ is a reciprocal lattice vector, determining the regular properties (short-range order) of the nonuniform medium. The scattering coefficients γ and the phase (v) and group (c) propagation velocities of electromagnetic waves corresponding to two roots of the dispersion relation are calculated. © *1995 American Institute of Physics.*

A great deal of attention is being devoted to problems involving wave propagation in nonuniform media.[1,2] The problem of solving the wave equation for the initial (in general, tensor[3,4]) field can usually be reduced to solving the corresponding equation (in some approximation[5]) for a scalar wave.[6]

In the present paper we solve the problem of the propagation of scalar waves in an unbounded, nonabsorbing nonuniform medium with short-range order. Spatial dispersion on a macroscopic scale is taken into account. The dynamic characteristics of the nonuniform medium are calculated by a method proposed in Refs. 3 and 4 and elaborated in Refs. 6 and 7. Attention is focused mainly on calculating the parameters of the mean field, which has the form of a monochromatic plane wave.

First, we generalize the expression for the binary correlation function of a completely disordered medium with sharp boundaries between grains of nonuniformity. The coordinate dependence of this function has the form[1,2]

$$\psi(\mathbf{r}_1,\mathbf{r}_2)\equiv\psi(\rho)=\exp(-\rho),\quad \rho\equiv\mathbf{r}/a\equiv(\mathbf{r}_1-\mathbf{r}_2)/a, \tag{1.1}$$

where a is the spatial correlation scale. Short-range order gives rise to damped oscillations of the correlation function with increasing values of its argument. The function

$$\varphi(\mathbf{r}_1,\mathbf{r}_2)\equiv\varphi(\rho)=\psi(\rho)\cos\mathbf{pr} \tag{1.2}$$

is the simplest function that takes into account the oscillatory damping of the correlation function while preserving the parity of the function. In what follows we employ a correlation function of the more general form

$$\varphi(\rho)=\psi(\rho)\cos\mathbf{b}\rho,\quad \mathbf{b}\equiv a\mathbf{p}, \tag{1.3}$$

where $\mathbf{p}$ is a reciprocal lattice vector, which determines the regular properties (short-range order) of the nonuniform medium. The physical meaning of the generalization (1.3) is that in the limit $a\to\infty$ the correlation function will be strictly periodic (which corresponds to a layered medium), and in the limit $b\to 0$ we arrive at the case (1.1) (completely disordered macroscopically isotropic medium with no short-range order).

2. DISPERSION RELATION

We consider a scalar monochromatic field $E(\mathbf{r},t)=E(\mathbf{r})\exp(-i\omega t)$ described by the Helmholtz equation

$$(\Delta+k_c^2\bar{\varepsilon})E(\mathbf{r})=0, \tag{2.1}$$

$$k_c^2\equiv\varepsilon_c\omega^2/c_0^2,\quad \bar{\varepsilon}\equiv\varepsilon/\varepsilon_c,\quad \varepsilon\equiv\varepsilon(\mathbf{r}). \tag{2.2}$$

For definiteness, we take the random scalar field ε to be the permittivity of the nonuniform medium. Then E will be the electric field strength, which is related to the induction D by $D=\varepsilon E$; k_c is the wave number in a uniform medium (comparison medium) with permittivity ε_c; and c_0 is the speed of light in free space.

Averaging Eq. (2.1) over a statistical ensemble of realizations (the average is denoted by the angular brackets) and introducing via the equation

$$\langle D\rangle=\langle\varepsilon E\rangle=\hat{\varepsilon}_*\langle E\rangle \tag{2.3}$$

the total effective permittivity operator $\hat{\varepsilon}_*$, we arrive at the Helmholtz equation

$$\hat{L}_*\langle E\rangle=0,\quad \hat{L}_*\equiv\Delta\hat{I}+k_c^2\hat{\bar{\varepsilon}}_*. \tag{2.4}$$

for the mean field $\langle E\rangle$. Here, $\hat{I}$ is the identity operator. To solve Eq. (2.4), it is necessary to find the explicit form of the operator $\hat{\bar{\varepsilon}}_*$. A method for doing this is described in, for example, Ref. 6. Here, we present the basic results required for our subsequent calculations.

Introducing the Green's operator $\hat{H}_c$ of the Helmholtz equation for the comparison medium

$$\hat{L}_c\hat{H}_c=-\hat{I},\quad \hat{L}_c\equiv(\Delta+k_c^2\varepsilon_c)\hat{I}, \tag{2.5}$$

we write the operator $\hat{\bar{\varepsilon}}_*$ in the pairwise interaction approximation

$$\hat{\bar{\varepsilon}}_*=\langle\bar{\varepsilon}\rangle\hat{I}+\langle\bar{\varepsilon}'\hat{Q}_c\bar{\varepsilon}'\rangle, \tag{2.6}$$

$$\hat{Q}_c\equiv k_c^2\hat{H}_c,\quad \bar{\varepsilon}'\equiv\bar{\varepsilon}-\langle\bar{\varepsilon}\rangle. \tag{2.7}$$

The required parameters of the mean field can be calculated using (2.6) together with Eq. (2.4). According to Eq. (2.6), only information about the pairwise (two-particle) interactions between the nonuniformities described by the random field $\varepsilon(\mathbf{r})$ is required to find $\hat{\bar{\varepsilon}}_*$. The approximation (2.6), written in terms of the operators $\hat{L}_*$ or $\hat{H}_* = -\hat{L}_*^{-1}$, is called the Bourret approximation.[1]

To calculate the parameters of the wave, we employ the dispersion relation

$$x^2 - q^2\bar{\varepsilon}_*(\mathbf{x},q) = 0, \quad \mathbf{x} \equiv a\mathbf{k}_*, \quad q \equiv ak_c, \tag{2.8}$$

corresponding to the integral equation (2.4) for the mean field $\langle E\rangle$, which has the form of a uniform plane wave:

$$\langle E(\mathbf{r})\rangle = E_0 \exp(i\mathbf{k}_*\mathbf{r}), \tag{2.9}$$

$$\mathbf{k}_* = k_*\mathbf{n}, \quad k_* \equiv k_1 + ik_2. \tag{2.10}$$

The function $\bar{\varepsilon}_*(\mathbf{x},q)$ is the Fourier transform, written in dimensionless variables, of the kernel $\bar{\varepsilon}_*(\mathbf{r},\omega)$ of the operator $\hat{\bar{\varepsilon}}_*$, and the spatial scale a of the correlations, which appears in Eqs. (1.1) and (2.8), is determined by the coordinate dependence of the two-point correlation function

$$\langle \bar{\varepsilon}'(\mathbf{r}_1)\bar{\varepsilon}'(\mathbf{r}_2)\rangle \equiv D_{\bar{\varepsilon}}\varphi(\mathbf{r}_1,\mathbf{r}_2), \quad D_{\bar{\varepsilon}} \equiv \langle(\bar{\varepsilon}')^2\rangle \tag{2.11}$$

of the random field $\bar{\varepsilon}(\mathbf{r})$, which here and below is assumed to be statistically homogeneous.[1,2]

The analysis given below is based on the investigation of the roots of the dispersion relation (2.8), which determine the parameters of the plane wave (2.9). In the approximation (2.6) for the function $\bar{\varepsilon}_*(\mathbf{x},q)$ we obtain

$$\bar{\varepsilon}_*(\mathbf{x},q) = \langle\bar{\varepsilon}\rangle + D_{\bar{\varepsilon}}F(\mathbf{x},q), \tag{2.12}$$

$$F(\mathbf{x},q) = \frac{1}{8\pi^3}\int \varphi(\mathbf{x}-\mathbf{y})Q_c(\mathbf{y},q)d\mathbf{y}. \tag{2.13}$$

Here, $\mathbf{y} \equiv a\mathbf{k}$ is the dimensionless wave vector, and the Fourier transform $Q_c(\mathbf{y},q)$ of the kernel of the operator $\hat{Q}_c$ from Eq. (2.7) has the form

$$Q_c(\mathbf{y},q) = q^2/(y^2 - q^2). \tag{2.14}$$

For direct calculations we employ the normalized two-point correlation function of the form (1.3) introduced in Eq. (2.11). The Fourier transform of the function (1.3), which is denoted by the same letter (with a different argument), is

$$\varphi(\mathbf{y}) = 0.5[\varphi_+(\mathbf{y}) + \varphi_-(\mathbf{y})], \tag{2.15a}$$

$$\varphi_\pm(\mathbf{y}) = 8\pi/[1 + (\mathbf{y}\pm\mathbf{b})^2]^2. \tag{2.15b}$$

Substituting Eq. (2.15) into Eq. (2.13), we find

$$F(\mathbf{x},q) = 0.5[F_+(\mathbf{x},q) + F_-(\mathbf{x},q)], \tag{2.16a}$$

$$F_\pm(\mathbf{x},q) = q^2/[(\mathbf{x}\pm\mathbf{b})^2 - (q+i)^2]. \tag{2.16b}$$

The choice of the arbitrary parameter ε_c is determined by the specific problem being solved. We used the condition

$$\langle\bar{\varepsilon}\rangle = 1 \Rightarrow \varepsilon_c = \langle\varepsilon\rangle, \quad D_{\bar{\varepsilon}} = D_\varepsilon\langle\varepsilon\rangle^{-2} \equiv D, \tag{2.17}$$

which simplifies the expressions (2.12) for $\bar{\varepsilon}_*$ and the roots of Eq. (2.8). To study small fluctuations, it is best to choose the quantity $D<1$ as a small parameter.

As follows from Eq. (2.16b), the parameters of the wave depend on the angle $\theta \equiv \arccos(\mathbf{xb}/xb)$ between the wave vector $\mathbf{x}$ and the reciprocal lattice vector $\mathbf{b}$. In the general case, the function F is

$$F = \frac{q^2[x^2+b^2-(q+i)^2]}{[x^2+b^2-(q+i)^2]^2 - (2xb\cos\theta)^2}. \tag{2.18a}$$

If, however, the wave propagates along the layers, then $\cos\theta = 0$ and the expression (2.18a) simplifies to

$$F = \frac{q^2}{x^2+b^2-(q+i)^2}. \tag{2.18b}$$

In the general case, the coordinate dependences (1.2) and (1.3) of the two-point correlation function (2.11) are too complicated to be able to solve the dispersion relation (2.8) analytically. Even for the simplest correlation function (1.1), the solution must be limited to approximations of this solution which refer to a limited range of wave numbers. It is convenient to classify them on the basis of the asymptotic solutions of Eq. (2.8) in the case of a disordered nonuniform medium described by the exponential function (1.1).

These ranges are as follows:[3,6]

l - long-wavelength range $\quad q \ll 1$, (2.19)

ls - transitional region $\quad q \approx q_{ls} \equiv 1$, (2.20)

s - short-wavelength range $\quad 1 < q < 1/\sqrt{D}$, (2.21)

su - transitional region $\quad 1 \leqslant q \approx q_{su} \equiv 1/\sqrt{D}$, (2.22)

u - ultrashort-wavelength range $\quad 1 < 1/\sqrt{D} < q$. (2.23)

We note that the asymptotic ranges (2.19) and (2.23) always hold, while the short-wavelength asymptotic range (2.21) is clearly defined only for small enough values of D.

3. DISCUSSION

We consider below some characteristics of the field (2.9), calculated on the basis of the dimensionless wave number x satisfying the dispersion relation (2.8) for a medium described by the effective permittivity $\bar{\varepsilon}_*$.

We introduce the dimensionless scattering coefficient as a quantitative measure of wave scattering

$$a\gamma \equiv \bar{\gamma} \equiv 2x_2, \quad x \equiv ak_* \equiv x_1 + ix_2, \tag{3.1}$$

where γ is the intensity damping coefficient of the wave.[1] The dimensionless velocities are given by

$$\bar{v} \equiv \frac{q}{x_1} = \frac{v_*}{v_c}, \quad \frac{1}{\bar{c}} \equiv \frac{dx_1}{dq} = \frac{v_c}{c_*},$$

$$c_0 \equiv v_c\sqrt{\varepsilon_c}, \tag{3.2}$$

where v_* and c_* are, respectively, the phase and group velocities of the monochromatic plane wave in a medium with the effective properties.

The correlation function (1.3) contains two parameters: the scalar parameter a (spatial scale of the correlations) and a vector parameter $\mathbf{p}$ (characterizing the short-range order). In the limit $a\to\infty$, the exponential approaches 1 and the correlation function is strictly periodic, which characterizes a layered medium. The other limiting case ($p\to 0$, $a\neq\infty$) corresponds to a completely disordered medium. In intermediate cases, the degree of ordering is determined by the ratio of a

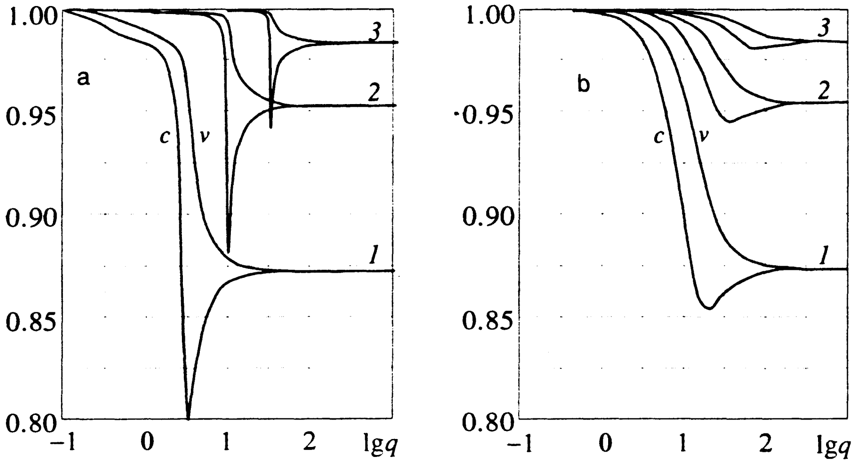

FIG. 1.

and $1/p$. One other parameter must be taken into account—the wave vector **k**, whose orientation relative to **p** strongly influences the dynamic properties of the inhomogeneous medium.

The solution of the dispersion relation (2.8) contains two roots, one of which gives in the long-wavelength limit Rayleigh's law for the scattering coefficient ($\propto$ (frequency)^4), while the other root is virtually independent of the frequency, although its contribution to scattering is negligible, as will be illustrated below. Keeping this in mind, we shall term the wave corresponding to the first root a real wave and the wave corresponding to the second root a virtual wave. Figures 1–2, discussed below, correspond to the function (2.18b), which describes wave propagation perpendicular to the vector **p**.

Figure 1 displays the phase velocity $\bar{v}$ and the group velocity $\bar{c}$ for a real wave as a function of the logarithm of the dimensionless wave number q. The numbers on the curves are the values of the parameter $n=-\log D$. Figure 1a refers to a completely disordered medium ($b=0$), and Fig. 1b refers to the case $b=10$. Comparing the graphs shows that short-range order affects mostly the dispersion of the group velocity. The dip in the group velocity becomes less pronounced as b increases, and in accordance with the well-known solutions,[8,9] the dip vanishes completely in the limit of a strictly periodic layered medium.

Figures 2a and 2b display the parameter $\nu \equiv d \log \gamma / d \log q$ as a function of the logarithm of the dimensionless wave number. The values $n=-\log D$ are indicated by the numbers on the curves. Figure 2a corresponds to a completely disordered medium ($b=0$), while Fig. 2b corresponds to the case $b=5$. If the scattering coefficient were a power-law function of the frequency, then the parameter ν would be the exponent. For the three asymptotic laws, the values of ν are 4, 2, and 0 (Rayleigh region, short wavelengths, and the geometrical optics region). The peaks correspond to the fact that the power-law approximation for the scattering cross section is incorrect near the transition from short wavelengths to ultrashort wavelength. Comparing Figs. 2a and 2b shows that short-range order results in narrowing (or vanishing) of the short-wavelength asymptotic range. For example, if for a completely disordered medium the $\nu=2$ asymptotic behavior is first observed at $n=3$, then in the presence of short-range order it is first observed only at $n=6$.

Comparing the $\log(q)$ dependences of the scattering coefficient of the real and virtual waves shows that the difference of the corresponding curves for the cases $b=0$ and $b=1$ is appreciable only for long wavelengths.

In the ranges (2.19)–(2.21), the contribution of the virtual component can be neglected. Moreover, the scattering coefficient of this wave is much greater than that of the real wave. These parameters become comparable for the two components only at the transition region (2.22). In this case, to calculate the wave process in a nonuniform medium, Bourret's approximation must be used and both waves must be taken into account. Comparing the frequency depen-

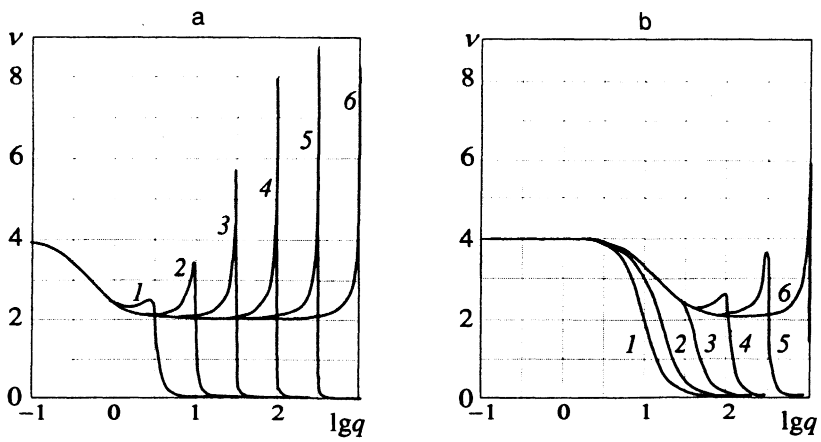

FIG. 2.

dences with the propagation velocities of the real and virtual waves shows that the phase and group velocities of the virtual wave, in contrast to the real wave, increase with increasing wave number, and instead of a dip, as in the case of a real wave, the group velocity of the virtual wave exhibits peaks near the transition from short to ultrashort wavelengths. The wavenumber dependences of the phase and group velocities are similar to the curves obtained by reflecting the curves for a real wave about the $\bar{v}=\bar{c}=1$ axis.

The calculations based on the solution of the dispersion relation (2.8) revealed that the effects observed in completely disordered random inhomogeneous media also occur in media with short-range order. The existence of short-range order greatly influences the shape of the curves of $\bar{v}$, $\bar{c}$, and $\bar{\gamma}$ as a function of $\log(q)$ only for short wavelengths (2.21), and less strongly for long wavelengths (2.19) and ultrashort wavelengths (2.23), where the well-known asymptotic laws for $\bar{\gamma}$ hold ($\bar{\gamma} \propto q^4$ and $\bar{\gamma}$=const, respectively).

This investigation was based on a calculation of the mean field in the Bourret approximation, which makes it possible to take into account macroscopic spatial dispersion (owing to the presence of nonuniformities of the medium) and to incorporate all wavelengths within the same approach. If, however, the spatial dispersion is neglected, then different computational schemes must be used in different ranges.[1,10–13] Note also that the mean-field calculation of the scattering coefficient $\bar{\gamma}$ gives a value which is somewhat too high.[14]

The results obtained can be used to describe wave propagation in randomly nonuniform media with short-range order. The characteristics of wave propagation in completely disordered media, described by an exponential correlation function of the material parameters, which is obtained from Eq. (1.3) by setting $b=0$, were studied in Refs. 1, 3, 6, 7, 10, 12, and 13. This situation is typical of one-phase polycrystals. For materials with a more complicated structure, such as multiphase polycrystals and composite materials, short-range order is always manifested, as a result of which the correlation function exhibits oscillatory damping. Such a coordinate dependence has been observed experimentally for fiber composite materials.[15,16]

If a multiphase polycrystal or composite material is macroscopically isotropic, then short-range order will be taken into account by the expression (1.3) with $\mathbf{b}\boldsymbol{\rho}=b\rho$. We note that a similar situation occurs at the molecular level in liquids, where short-range order also shows up.[17] Another limiting case corresponds to $b=\text{const}\neq 0$, where we obtain a stochastic medium with short-range order in the case $\boldsymbol{\rho}\|\mathbf{b}$ and a uniform medium in the case $\boldsymbol{\rho}\perp\mathbf{b}$. The latter case corresponds to a stochastic layered medium, in which the alternation of layers exhibits short-range order.

In summary, our results describe a wide class of materials which possess stochastic structure and which can be macroscopically isotropic as well as anisotropic.

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