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Waves in a superlattice with anisotropic inhomogeneities

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Dependences of the dispersion laws and damping of waves in an initially sinusoidal superlattice on inhomogeneities with anisotropic correlation properties are studied for the first time. The period of the superlattice is modulated by the random function described by the anisotropic correlation function $K_\phi(\mathbf{r})$ that has different correlation radii, $k_{\parallel}^{-1}$ and $k_{\perp}^{-1}$, along the axis of the superlattice z and in the plane xy, respectively. The anisotropy of the correlation is characterized by the parameter $\lambda = 1 - k_\perp/k_\parallel$ that can change from $\lambda = 0$ to $\lambda = 1$ when the correlation wave number $k_\perp$ changes from $k_\perp = k_\parallel$ (isotropic 3D inhomogeneities) to $k_\perp = 0$ (1D inhomogeneities). The correlation function of the superlattice $K(\mathbf{r})$ is developed. Its decreasing part goes to the asymptote L that divides the correlation volume into two parts characterized by finite and infinite correlation radii. The dependences of the width of the gap in the spectrum at the boundary of the Brillouin zone $\Delta\nu$ and the damping of waves ξ on the value of λ are studied. It is shown that decreasing L leads to the decrease of $\Delta\nu$ and increase of ξ with the increase of λ.

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1. Theoretical studies of the wave spectrum in disordered superlattices (SLs) have been carried out very intensively in recent years. This is due to the wide use of these materials in various high technology devices as well as to the fact that they are convenient models for developing new methods of theoretical physics for studying media without translation symmetry. Several methods exist now for developing a theory of such SLs: the modeling of the randomization by altering the order of successive layers of two different materials [1 – 7]; the numerical modeling of the random derivations of the interfaces between layers from their initial periodic arrangement [8 – 10]; the postulating of the form of the correlation function of a SL with inhomogeneities [11,12]; the application of the geometrical optics approximation [13]; the development of the dynamic composite elastic medium theory [14].

One more method for investigating the influence of inhomogeneities on the wave spectrum of a SL was suggested in Ref. [15], the method of the random spatial modulation (RSM) of the period of the SL. This method is an extension of the well-known theory of the random frequency (phase) modulation of a radio signal [16, 17] to the case of spatial inhomogeneities in a SL. The advantage of this method is that the form of the correlation function (CF) of the SL is not postulated but is developed from the most general assumptions about the nature of a random spatial modulation of the SL period. The knowledge of the CF corresponding to a particular type and dimensionality of inhomogeneities permitted applying the methods of investigations of averaged Green functions to find the energy spectrum and other characteristics of the waves [15, 18 – 25]. In all these papers only isotropic 3D inhomogeneities were considered side by side with 1D inhomogeneities.

In the present paper effects of 3D inhomogeneities with anisotropic correlation properties on the wave spectrum of SLs is studied for the first time. The continuous transition between isotropic 3D inhomogeneities and 1D inhomogeneities as the anisotropy of the correlations is changed is considered.

2. Correlation Function. A SL is characterized by the dependence of some material parameter A on the coordinates $\mathbf{x} = \{x, y, z\}$. The physical nature of the parameter $A(\mathbf{x})$ can be different. This parameter can be a density of matter or a force constant for the elastic system of a medium, the magnetization, anisotropy, or exchange for a magnetic system, and so on. We represent $A(\mathbf{x})$ in the form

$$A(\mathbf{x}) = A\,[1 + \gamma\rho(\mathbf{x})]\,, \qquad (1)$$

where A is the average value of the parameter, γ is its relative rms variation, and $\rho(\mathbf{x})$ is a centered ($\langle\rho(\mathbf{x})\rangle = 0$) and normalized ($\langle\rho(\mathbf{x})^2\rangle = 1$) function. The function $\rho(\mathbf{x})$ describes the periodic dependence of the parameter along the SL axis z, as well as the random spatial modulation of this parameter which, in the general case, can be a function of all three coordinates $\mathbf{x} = \{x, y, z\}$.

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We will consider in this paper a SL that has a sinusoidal dependence of the material parameter on the coordinate z in the initial state when inhomogeneities are absent. According to the RSM method we represent the function $\rho(\mathbf{x})$ in the form

$$\rho(\mathbf{x}) = \sqrt{2}\cos\left[q(z - u(\mathbf{x})) + \psi\right], \tag{2}$$

where $q = 2\pi/l$ is the SL wave number, l is its period, and $u(\mathbf{x})$ is the random spatial modulation. The SL is characterized by the CF $K(\mathbf{r}) = \langle\rho(\mathbf{x})\rho(\mathbf{x}+\mathbf{r})\rangle$ the general form of which was obtained in Ref. [15]:

$$K(\mathbf{r}) = \cos\ qr_z \exp\left[-\frac{1}{2}Q(\mathbf{r})\right]. \tag{3}$$

Here

$$Q(\mathbf{r}) = \frac{2q^2}{(2\pi)^3}\int\int K_\varphi(\mathbf{r}_1)e^{-i\mathbf{k}\mathbf{r}_1} \times \times (1 - \cos\ \mathbf{k}\mathbf{r})\frac{d\mathbf{k}}{k^2}d\mathbf{r}_1, \tag{4}$$

where $K_\varphi = \langle\varphi(\mathbf{x})\varphi(\mathbf{x}+\mathbf{r})\rangle$ is the CF of the function $\varphi = \text{grad}\ u(\mathbf{x})$.

Upon integrating Eq.(4) with respect to $\mathbf{k}$, we obtain $Q(\mathbf{r})$ in the form

$$Q(\mathbf{r}) = \frac{q^2}{4\pi}\int K_\varphi(\mathbf{r}_1)\left[\frac{2}{|\mathbf{r}_1|} - \frac{1}{|\mathbf{r}_1 - \mathbf{r}|} - \frac{1}{|\mathbf{r}_1 + \mathbf{r}|}\right]d\mathbf{r}_1. \tag{5}$$

On the assumption that the correlation properties of the function $u(\mathbf{x})$ are isotropic in the xy plane and anisotropic in the directions between the z axis and the xy plane, we model the CF in the form:

$$K_\varphi(\mathbf{r}) = \sigma^2 \exp\left\{-\frac{1}{2}\left[k_\perp^2(r_x^2 + r_y^2) + k_\parallel^2 r_z^2\right]\right\}, \tag{6}$$

where $k_\perp$ and $k_\parallel$ are the correlation wave numbers in the xy plane and along the z axis, respectively. This function in the 1D ($k_\perp = 0$), 2D ($k_\parallel = 0$), or isotropic 3D ($k_\perp = k_\parallel$) limit transforms into the Gaussian function. It was shown in Ref. [21] that the coefficient σ in Eq. (6) has the form

$$\sigma = \gamma_u(k_\parallel^2 + 2k_\perp^2)^{1/2}\Big/ q. \tag{7}$$

Substituting Eq. (6) into Eq. (5) we obtain a complicated expression where only one integration can be performed in the threefold integral. For overcoming this difficulty we obtain one more representation of the function $Q(\mathbf{r})$. Using the following integral representation [27]

$$\frac{1}{r} = \sqrt{\frac{2}{\pi}}\int_0^\infty \exp(-r^2t^2/2)dt, \tag{8}$$

where the integration variable t has the dimensionality of $[r]^{-1}$, we obtain $Q(\mathbf{r})$ in the form

$$Q(\mathbf{r}) = \frac{q^2}{(2\pi)^{3/2}}\int_{-\infty}^{\infty} d\mathbf{r}_1 \int_0^\infty dt K_\varphi(\mathbf{r}_1) \times \times (2e^{-t^2 r_1^2/2} - e^{-t^2(\mathbf{r}_1 - \mathbf{r})^2/2} - e^{-t^2(\mathbf{r}_1 + \mathbf{r})^2/2}). \tag{9}$$

The integral with respect to $\mathbf{r}_1$ can be performed exactly in this fourfold integral after substituting K_φ in the form of Eq. (6) into it. As a result, we obtain $Q(\mathbf{r})$ in the form a one-dimensional integral with respect to τ:

$$Q(\mathbf{r}) = 2\gamma_u^2(1 + 2\varkappa^2)\int_0^\infty\left(\frac{1}{(\varkappa^2 + \tau^2)\sqrt{1 + \tau^2}} - \frac{\exp\left\{-\frac{(k_\parallel r\tau)^2}{2}\left[\frac{\varkappa^2\sin^2\theta}{\varkappa^2 + \tau^2} + \frac{\cos^2\theta}{1 + \tau^2}\right]\right\}}{(\varkappa^2 + \tau^2)\sqrt{1 + \tau^2}}\right)d\tau, \tag{10}$$

where $\tau = t/k_\parallel$ is a dimensionless variable, and $\cos\theta = r_z/r$, $\varkappa = k_\perp/k_\parallel$.

For the limiting cases of 1D ($\varkappa = 0$), 2D ($\varkappa \to \infty$), and isotropic 3D ($\varkappa = 1$) inhomogeneities this integral can be calculated exactly and we obtain known formulas [15]. In the general case of an arbitrary value of $\varkappa$ the approximation of Eq. (10) by a simpler expression must be done for analytical calculations. For the selection of this expression we calculate $Q(\mathbf{r})$ at $r = 0$ and $r \to \infty$. The integral in Eq. (10) is calculated exactly at both of these limits, and we obtain, respectively,

$$Q_0(\mathbf{r}) = \gamma_u^2\frac{1 + 2\varkappa^2}{1 - \varkappa^2}\{F(\varkappa) - \varkappa^2 + \left[2 + \varkappa^2 - 3F(\varkappa)\right]\cos^2\theta\}(k_\parallel r)^2,$$
$$Q_\infty = 2\gamma_u^2\frac{1 + 2\varkappa^2}{\varkappa^2}F(\varkappa), \tag{11}$$

where

$$F(\varkappa) = \frac{\varkappa}{\sqrt{1 - \varkappa^2}}\arctan\frac{\sqrt{1 - \varkappa^2}}{\varkappa}. \tag{12}$$

Using these expressions and extending the idea that has been suggested in Ref. [23] for the approximation of the CF of isotropic 3D inhomogeneities, we suggest the approximation formula for the CF of the anisotropic inhomogeneities in the form

$$K(\mathbf{r}) = \cos qr_z\left\{L + (1 - L)e^{-Pr}\right\}, \tag{13}$$

where L is the asymptote of the decreasing part of $K(\mathbf{r})$ determined by the equation

$$L = \exp(-\frac{1}{2}Q_\infty); P = Q_0(r)/k_\parallel r^2. \tag{14}$$

In the present work we restrict ourselves to the consideration of uniaxial anisotropic inhomogeneities for which the values of $\varkappa$ are between 0 and 1. It is convenient to introduce the parameter of the uniaxial anisotropy $\lambda = 1 - \varkappa$, whose values are also between 0 and 1. In this case $\lambda = 0$ corresponds to the isotropic 3D inhomogeneities and $\lambda = 1$ corresponds to the inhomogeneities with the maximum value of the anisotropy, namely 1D inhomogeneities.

For the isotropic 3D inhomogeneities considered in Ref. [23] the value of the asymptote L depended only on the rms fluctuation γ_u. For the anisotropic inhomogeneities the asymptote L according to Eq. (14) depends on γ_u as well on the parameter anisotropy λ (Fig.1). One can see that L decreases with the increase of γ_u or λ;

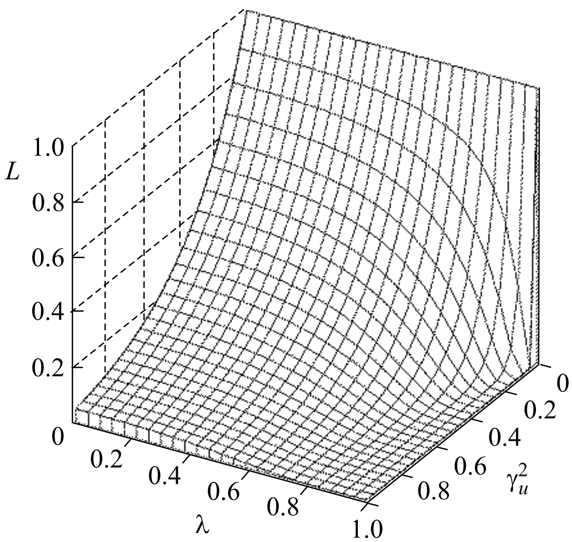

Fig.1. Dependence of the asymptote L of the CF on the rms fluctuation γ_u and the anisotropy parameter of the correlations λ

the value of L goes to zero at the point of the transition of the system from 3D to 1D dimensionality.

3. Dispersion law and damping of waves. We consider the equation for waves in the superlattice in the form

$$\nabla^2\mu + (\nu - \epsilon\rho(\mathbf{x}))\mu = 0, \tag{15}$$

where the expressions for the parameters ϵ and ν, and the variable μ are different for waves of different natures. For spin waves, when the parameter of the superlattice $A(\mathbf{x})$ in Eq. (1) is the value of the magnetic anisotropy $\beta(\mathbf{x})$, we have [15] $\nu = (\omega - \omega_0)/\alpha g M$, $\epsilon = \gamma\beta/\alpha$, where ω is the frequency, $\omega_0 = g(H + \beta M)$, g is the gyromagnetic ratio, α is the exchange parameter, H is the magnetic field strength, M is the value of the magnetization, β is the average value of the anisotropy, and γ is its relative rms variation. For elastic waves in the scalar approximation we have $\nu = (\omega/v)^2$, $\epsilon = \gamma\nu$, where γ is the rms fluctuation of the density of the material and v is the wave velocity. For electromagnetic waves in the same approximation we have $\nu = \epsilon_e(\omega/c)^2$, $\epsilon = \gamma\nu$, where ϵ_e is the average value of the dielectric permeability, γ is its rms deviation, and c is the speed of light.

Laws of the dispersion and damping of the averaged waves are determined by the equation for the complex frequency $\nu = \nu' + i\xi$, which follows from the vanishing of the denominator of the Green function of Eq.(15). In the Bourret approximation [28] this equation can be represented in the form [21]

$$\nu - k^2 = -\frac{\epsilon^2}{4\pi}\int K(\mathbf{r})\exp\left[-i(\mathbf{kr} + \sqrt{\nu}r)\right]\frac{d\mathbf{r}}{r}. \tag{16}$$

Substituting Eq. (13) in Eq. (16) we calculate this integral exactly. As a result, we obtain a complicated equation that we do not give here. When the conditions

$$\gamma_u^2 k_\| \ll |\sqrt{\nu}|, \qquad \Lambda \ll |\nu| \tag{17}$$

are satisfied, this equation can be reduced to a cubic equation,

$$\nu - k^2 = \frac{\Lambda^2}{4}\Big\{\frac{L}{\nu - (k-q)^2} + \\ + (1-L)\frac{1 - i\gamma_u^2 k_\| f_1\sqrt{\nu}/(k-q)^2}{\left[\sqrt{\nu} - \gamma_u^2 k_\|(f_0 + f_1)\right]^2 - (k-q)^2}\Big\}, \tag{18}$$

where

$$\Lambda = \epsilon/\sqrt{2},$$
$$f_0 = \frac{1+\varkappa^2}{2(1-\varkappa^2)}\left[F(\varkappa) - \varkappa^2\right],$$
$$f_1 = \frac{1+\varkappa^2}{2(1-\varkappa^2)}\left[2 + \varkappa^2 - 3F(\varkappa)\right]. \tag{19}$$

In the limiting cases $\lambda = 1$ and $\lambda = 0$ Eq. (18) transforms into equations for 1D and isotropic 3D inhomogeneities obtained earlier in Refs. [15, 23], respectively.

Equation (18) has been investigated by numerical methods. The results of these investigations are shown in Fig.2. Fig.2a shows the behavior of the width of the gap at the Brillouin zone boundary $\Delta\nu = \nu'_+ - \nu'_-$ with the increase of the anisotropy parameter λ for several values of γ_u^2, that are depicted at the corresponding curves. One can see that the maximum values of the width of the gap (which are different for different γ_u^2) correspond to isotropic 3D inhomogeneities ($\lambda = 0$). With the increase of the anisotropy parameter λ the width of the gap decreases, with this decrease becoming nonmonotonic in the region $\lambda \gtrsim 0.8$. Even some

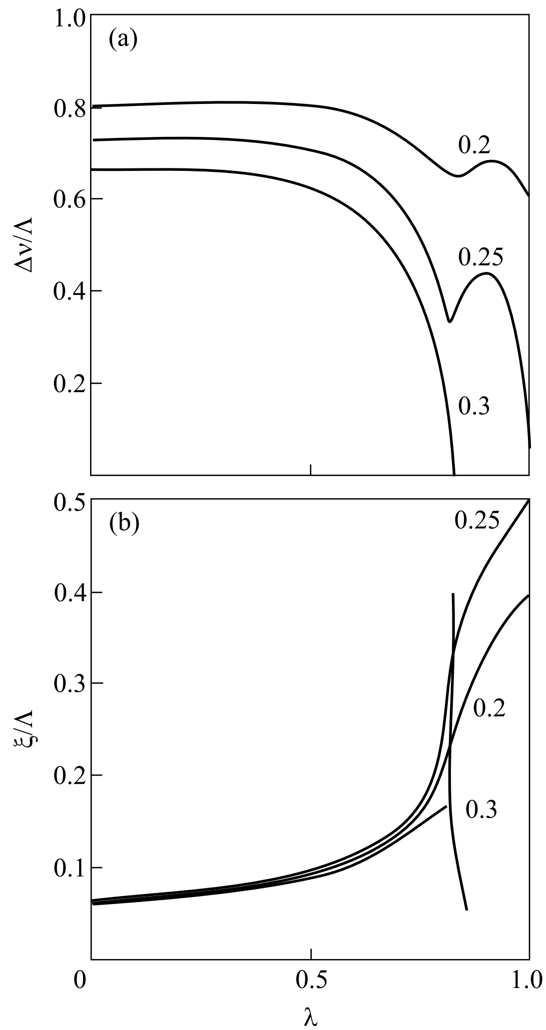

Fig.2. Dependence of the width of the gap (a) and damping of the waves (b) at the Brillouin zone boundary on the value of the anisotropy of correlations λ for different values of γ_u^2 depicted at the corresponding curves. All graphs correspond to the same normalized correlation number $\eta = k_{\|} q/\Lambda = 4$

increase of $\Delta\nu$ takes place in this region which changes again to a decrease when λ goes to unity. For $\gamma_u^2 > 0.25$ the closing of the gap occures at some critical value of the anisotropy λ_c.

In Fig.2b the dependences of the damping $\xi_\pm$ at the Brillouin zone boundary on the parameter of the anisotropy λ are shown for the same values of γ_u^2. The minimum values of the damping correspond to the isotropic 3D inhomogeneities. The damping increases with the increase of the anisotropy and reaches the largest value for 1D inhomogeneities ($\lambda = 1$). For the curve with $\gamma_u^2 = 0.3$ at the critical point $\lambda = \lambda_c$, corresponding to the closing of the gap, the degeneracy of the real parts of the eigenfrequencies takes place ($\nu'_+ = \nu'_-$) and, correspondingly, the removal of the degeneracy of the damping [15]: $\xi_+ \neq \xi_-$ at $\lambda > \lambda_c$.

4. Conclusions. The limiting cases of our general model are the isotropic 3D inhomogeneities ($\lambda = 0$) and 1D inhomogeneities ($\lambda = 1$) that have been investigated in the framework of the RSM method earlier [15, 23]. It was shown in Ref. [25] that the main difference between the CFs for isotropic 3D and 1D inhomogeneities was that the decreasing function went to zero when $r \to \infty$ in the 1D case while the decreasing function in the isotropic 3D case went to the nonzero asymptote $L = \exp(-3\gamma_u^2)$. Because of this the 1D inhomogeneities had a finite correlation radius in the entire volume of the superlattice, while for the isotropic 3D case volumes with a finite correlation radius existed side by side with volumes with an infinite correlation radius. In Ref. [25] attention was also paid to the important role of the value of the asymptote L in the transition from the disordered SL to an ideal periodic one with the decrease of γ_u. In the 1D case this transition was carried out by increasing the correlation radius. For the 3D case another kind of transition took place: the changing of the relationship between the volumes with finite and infinite correlation radii went on in parallel with the increase of the correlation radius.

For the general case of anisotropic inhomogeneities the asymptote L depends not only on γ_u but also on λ. The changing of λ from 0 to 1 at $\gamma_u = \text{const}$ leads to the changing of L from $L = \exp(-3\gamma_u^2)$ to $L = 0$. Hence, the changing of the anisotropy parameter λ leads to two contributions to the changing of the form of the CF, exerting opposite influences on the characteristics of the wave spectrum. The increase of the correlation radius in the xy plane at the unchangeable correlation radius along z axis means the increase of the mean correlation radius of the system, that is the decrease of the disorder. This factor in itself could lead to the increase of the width of the gap $\Delta\nu$ at the Brillouin zone boundary and to the decrease of the damping ξ with the increase of λ. However, the increase of λ leads simultaneously to the decrease of L and, consequently, to the decrease of the correlation volume with an infinite correlation radius and to the increase of the volume with finite correlation radii. This factor must lead to the increase of the mean disorder in the system and, consequently, to the decrease of $\Delta\nu$ and increase of ξ. Simultaneous actions of both of these factors lead to the dependences of $\Delta\nu$ and ξ on λ depicted in Figs.2a and 2b. It is seen that the effects of the increase of the disorder prevail, and the decrease of $\Delta\nu$ and increase of ξ occur with the increase of λ. However, the struggle between the opposite factors leads to the appearance of a nonmonotonic dependence of $\Delta\nu$ on λ: even some increase of $\Delta\nu$ takes place in the region

$\lambda > 0.8$ that changes again to a decrease when λ goes to the unit.

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