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Waves in a Superlattice with Arbitrary Interlayer Boundary Thickness

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Abstract—The transmittance $D(\omega)$, reflectance $R(\omega)$, and dispersion $\omega(k)$ are investigated for waves of various nature propagating through a one-dimensional superlattice (multilayer structure) with arbitrary thickness of the interlayer boundary. The dependences of the band gap widths $\Delta\omega_m$ and their positions in the wave spectrum of the superlattice on the interlayer boundary thickness d and the band number m are calculated. Calculations are performed in terms of the modified coupled-mode theory (MCMT) using the frequency dependence of $R(\omega)$, as well as in the framework of perturbation theory using the function $\omega(k)$, which made it possible to estimate the accuracy of the MCMT method; the MCMT method is found to have a high accuracy in calculating the band gap widths and a much lower accuracy in determining the gap positions. It is shown that the m dependence of $\Delta\omega_m$ for electromagnetic (or elastic) waves is different from that for spin waves. Furthermore, the widths of the band gaps with $m = 1$ and 2 are practically independent of d, whereas the widths of all gaps for $m > 2$ depend strongly on d. Experimental measurements of these dependences allow one to determine the superlattice interface thicknesses by using spectral methods. © *2004 MAIK "Nauka/Interperiodica".*

1. INTRODUCTION

Propagation of waves of various nature (electromagnetic, elastic, spin, etc.) and their spectra in media with one-dimensional periodic modulation of the material parameters—multilayer structures or superlattices (SLs)—has been investigated theoretically in numerous studies. This problem is discussed in monographs [1–5] and reviews [6, 7]. The dispersion laws and wave propagation factors in SLs are determined to a large degree by the geometry of the modulation profile of the material parameters of the SLs. As a rule, rectangular and sinusoidal spatial modulations of parameters have been considered in the literature. Rectangular modulation corresponds to the case of maximally sharp boundaries between the SL layers (zero boundary thickness), and sinusoidal modulation corresponds to the limiting case of maximally smooth boundaries (the "boundary" thickness is equal to the "layer" thickness). A model with a rectangular modulation profile has been widely used when studying electromagnetic [8–11], elastic [12–16], and spin [17–22] waves. Waves of various physical nature for the model with a sinusoidal modulation profile of the material parameters were investigated in [23, 24]. In [25], spin waves were considered for both cases.

However, in real SLs, the modulation profile of the material parameters can be intermediate between these two limiting cases. For this reason, a model of an SL was proposed in [26] in which modulation is proportional to the Jacobian elliptic sine:

$$\rho(z) = \kappa\left(\frac{\mathbf{K}}{\mathbf{K}-\mathbf{E}}\right)^{1/2}\mathrm{sn}\left(\frac{\pi z}{2d}\right), \qquad (1)$$

where $d = \pi l/8\mathbf{K}$ is the SL interlayer boundary thickness; l is the SL period ($l/2 - d$ is the layer thickness); $\mathbf{K}$ and $\mathbf{E}$ are the complete elliptic integrals of the first and second kind, respectively; and κ is the modulus of these elliptic integrals. The factor before the elliptic sine corresponds to the normalization $\langle\rho^2(z)\rangle = 1$ (angle brackets mean averaging over the period l). The general form of function (1) is shown in Fig. 1. Depending on the modulus κ, this function describes the limiting

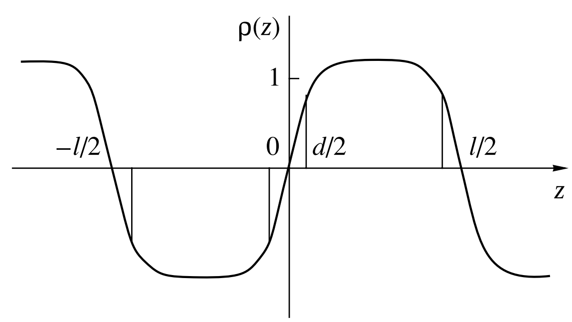

Fig. 1. Function given by Eq. (1) for $\kappa = 0.994$ ($d/l = 0.218$).

cases of a rectangular profile ($d/l = 0$, $\kappa = 1$, $\mathbf{K} = \infty$), a sinusoidal profile ($d/l = 1/4$, $\kappa = 0$, $\mathbf{K} = \pi/2$), and all intermediate values d/l. In Eq. (1), the boundary thickness d is determined such that the main variation in the material parameter occurs over the distance d for all values of d/l (Fig. 1). The basic feasibility of spectral methods of studying the boundary structure in SLs was demonstrated in [26]. In order to realize such methods, the theory needs to be extended in several directions. The present study deals with two of these directions. One of them is related to the fact that in [26] the spectrum of standing waves was calculated, while, in experiments with standing waves, only the wave dispersion law is studied directly. The other parameters (the reflectance and transmittance) are measured in experiments with traveling waves. Therefore, it is necessary to analyze the case of propagating waves for the model proposed in [26]. In the second direction of study, one should develop a more exact theory in order to find the dispersion law of waves for such a model. Both directions require the application and development of appropriate approximate methods of calculation, since the second-order equation with a coefficient whose coordinate dependence is described by an elliptic sine belongs to the general class of Hill equations and cannot be reduced to any well-known equations of this class. In particular, this equation cannot be reduced to the Lamé equation, which contains an elliptic sine squared.

2. WAVE PROPAGATION IN SUPERLATTICES

By way of example, we consider the propagation of electromagnetic waves in an SL with permittivity periodically modulated along the z axis:

$$\epsilon(z) = \epsilon'[1 - \gamma\rho(z)] - i\epsilon''. \quad (2)$$

Here, ϵ' and ϵ'' are the static components of the real and imaginary parts of the permittivity, respectively; γ is the relative root-mean-square modulation of the real part of the permittivity; and $\rho(z)$ is a periodic function with period l satisfying the conditions $\langle\rho(z)\rangle = 0$ and $\langle\rho^2(z)\rangle = 1$. We restrict ourselves to weakly perturbed media; i.e., we set $\gamma \ll 1$. We also assume that the order of magnitude of the ϵ''/ϵ' ratio does not exceed γ. We are interested in the solutions to the system of Maxwell equations near the frequencies of the Bragg resonances corresponding to the boundaries of the mth Brillouin zones. We consider waves propagating along the z axis. To find an approximate solution, we use the modified coupled-mode theory (MCMT) (see [27] and review [7]; the development of the application of the MCMT to optical waveguides is reviewed in [28]; originally, the coupled-mode theory was suggested in [29]). In this theory, a system of equations for the amplitudes of two

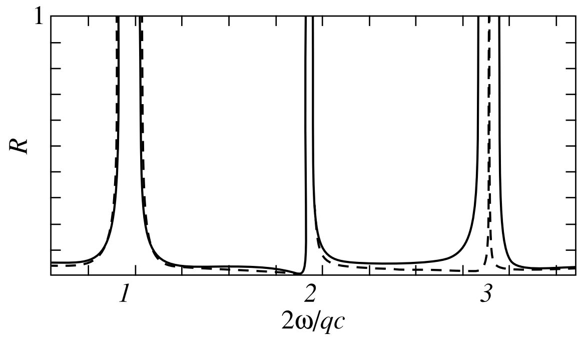

Fig. 2. $R(\omega)$ dependence for a semi-infinite SL near the first three Brillouin zones for rectangular (solid curve) and sinusoidal (dashed curve) modulations of the SL.

waves propagating in opposite directions is written out. The coupling parameters $\kappa_m^{\pm}$ in this system can be written as

$$\kappa_m^{\pm} = \frac{1}{4l}\int_0^l \frac{dz}{\epsilon(z)}\frac{d\epsilon(z)}{dz}\exp(\pm 2i\psi(z) \mp 2i\omega\tilde{n}z/c \pm imqz)$$
$$+ \frac{1}{4l}\sum_{j=1}^{N}\ln\frac{\epsilon(z_j+0)}{\epsilon(z_j-0)}\exp(\pm 2i\psi(z_j) \mp 2i\omega\tilde{n}z_j/c \pm imqz_j), \quad (3)$$

where $\psi(z) = \frac{\omega}{c}\int_0^l\sqrt{\epsilon(z')}dz'$, $\tilde{n} = c\psi(l)/\omega l$, $q = 2\pi/l$, the principal value of the integral is implied, and the sum takes into account the contribution of the permittivity jumps at discontinuity points z_j. Relation (3) is the main result of the MCMT, since all measured physical quantities, in particular, the reflectance $R(\omega)$ and transmittance $D(\omega)$, can be expressed in terms of the coupling parameters $\kappa_m^{\pm}$ (see, for example, [7]).

Figure 2 shows the frequency dependence of the reflectivity R calculated for a semi-infinite medium ($L \longrightarrow \infty$) in the absence of absorption ($\epsilon'' = 0$) for two well-known cases of limiting values of the boundary thickness: $d/l = 0$ (the case of a rectangular SL profile, represented by the solid curve in Fig. 2) and $d/l = 1/4$ (the case of a sinusoidal SL profile, represented by the dashed curve). The $R(\omega)$ dependence is plotted in the vicinity of three Brillouin zones, $m = 1$, 2, and 3. We see that the band gap widths are practically equal in the two limiting cases for both $m = 1$ and 2. However, for $m = 3$, these widths differ substantially. We intend to use this difference to construct the theoretical foundation for experimental determination of the boundary thickness d from spectral measurements. To this end, we must, first of all, obtain the dependence of the coupling parameters $\kappa_m^{\pm}$ on the SL parameters. Assuming that the function $\rho(z)$ in Eq. (2) has no discontinuities, we retain in Eq. (3) only the integral, into which we substitute the Fourier expansion of this function. If the gap number m is such that $m\gamma/2 \ll 1$, then the integrand in Eq. (3) can be expanded in powers of the small parameter γ. Keeping terms of up to the order of γ^3 and integrating, we obtain

$$\begin{aligned}\kappa_m^{\pm} = \pm\frac{imq}{8}e^{\pm i\Phi}\Bigg[&2\gamma\left(1 + i\frac{\epsilon''}{\epsilon'} - \frac{\epsilon''^2}{\epsilon'^2}\right)\rho_{\mp m}\\ &+ \gamma^2\left\{\frac{2\omega\sqrt{\epsilon'}}{mqc}\left(1 + \frac{3i}{2}\frac{\epsilon''}{\epsilon'}\right)\sum_n \frac{\mp m - n}{n}\rho_n\rho_{\mp m - n}\right.\\ &\left.+ \left(1 + 2i\frac{\epsilon''}{\epsilon'}\right)\sum_n \rho_n\rho_{\mp m - n}\right\}\\ &+ \gamma^3\left\{\frac{\omega\sqrt{\epsilon'}}{2mqc}\sum_{n+p\neq 0}\frac{\mp m - n - p}{n + p}\rho_n\rho_p\rho_{\mp m - n - p}\right.\\ &+ \sum_{n,p}\left(\mp\frac{\omega^2\epsilon'}{mq^2c^2}\frac{\mp m - n - p}{np} + \frac{\omega\sqrt{\epsilon'}}{mqc}\frac{\mp m - p}{p} + \frac{2}{3}\right)\\ &\left.\times\rho_n\rho_p\rho_{\mp m - n - p}\right\} + \dots\Bigg],\end{aligned} \tag{4}$$

where

$$\begin{aligned}\Phi = \frac{\omega\sqrt{\epsilon'}}{iqc}\Bigg[&\left(1 + \frac{i}{2}\frac{\epsilon''}{\epsilon'}\right)\gamma\sum_n\frac{\rho_n}{n}\\ &+ \frac{1}{4}\gamma^2\sum_{n+p\neq 0}\frac{\rho_n\rho_p}{n + p} + \dots\Bigg].\end{aligned} \tag{5}$$

After substituting Eq. (4) into the corresponding expressions for the transmittance D and reflectance R, their ω dependences can generally be constructed for any modulation profile and any thickness L of the SL. Using the $D(\omega)$ or $R(\omega)$ dependences, we can find, in particular, the gap widths at the boundaries of the Brillouin zones as functions of the interface thickness.

Let us obtain the explicit dependences of the gap widths on d for a simpler model of a semi-infinite SL in a nonabsorbing medium. In this case, in the region of band gaps, the function $R(\omega)$ has flat tops with $R = 1$. Using this condition, we obtain equations for the frequencies $\omega_m^{\pm}$ bounding the mth band gap:

$$\omega_m^{\pm} = \frac{c}{\tilde{\tilde{n}}}\left(\frac{mq}{2} \pm \left|\kappa_m^{+}\kappa_m^{-}\right|^{1/2}\right). \tag{6}$$

In these equations, the coefficients $\kappa_m^{\pm}$ depend on $\omega_m^{\pm}$. By solving these equations, we can find the width of the mth band gap $\Delta\omega_m = \omega_m^{+} - \omega_m^{-}$. We set $\epsilon'' = 0$ in Eq. (4) and substitute $\kappa_m^{\pm}$ defined by these expressions into Eqs. (6). By solving the obtained equations for $\omega_m^{\pm}$ to within the terms of the order of γ^3, we obtain

$$\begin{aligned}\omega_m^{\pm} = \frac{mqc}{2\sqrt{\epsilon'}}\Bigg[&1 + \frac{1}{8}\gamma^2\\ &\pm\frac{1}{16}\gamma^3\left(|\rho_m| \mp \sum_{n+p\neq 0}\rho_n\rho_p\rho_{-n-p}\right)\\ &\pm\left|\frac{1}{2}\rho_m\gamma + \frac{m}{4}\gamma^2\sum_p\frac{\rho_p\rho_{m-p}}{p} \pm \frac{m}{8}|\rho_m|\gamma^3\right.\\ &\left.\times\sum_p\frac{\rho_p\rho_{m-p}}{p} + \frac{1}{16}\gamma^3 S_m\right|\Bigg],\end{aligned} \tag{7}$$

where

$$\begin{aligned}S_m = &\sum_{n+p\neq 0}\frac{m - n - p}{n + p}\rho_n\rho_p\rho_{m-n-p}\\ &+ \sum_{n,p}\left(\frac{m^2}{np} + \frac{2}{3}\right)\rho_n\rho_p\rho_{m-n-p}.\end{aligned} \tag{8}$$

From these expressions, the gap widths can be found to be (to within terms of the order of γ^2)

$$\Delta\omega_m = \frac{mqc}{2\sqrt{\epsilon'}}\left|\rho_m\gamma + \frac{m}{2}\gamma^2\sum_p\frac{\rho_p\rho_{m-p}}{p}\right|. \tag{9}$$

Expressions (7)–(9) are valid for any shape of the SL profile $\rho(z)$ represented by the Fourier harmonics ρ_n in them.

Let us consider the functions having the so-called symmetry of the third kind [30],

$$\rho(z + l/2) = -\rho(z). \tag{10}$$

For all functions of this class, the Fourier harmonics ρ_n vanish for even n. Using this property, we can simplify Eqs. (7):

$$\omega_m^{\pm} = \frac{mqc}{2\sqrt{\epsilon'}} \times \begin{cases} 1 + \frac{1}{8}\gamma^2 + \pm\left|\frac{\rho_m}{2}\gamma + \frac{S_m}{16}\gamma^3\right| \pm \frac{|\rho_m|}{16}\gamma^3, & \text{for odd } m \\ 1 + \frac{1}{8}\gamma^2 \pm \frac{m}{4}\gamma^2\left|\sum_p \frac{\rho_p\rho_{m-p}}{p}\right|, & \text{for even } m. \end{cases} \quad (11)$$

The gap widths at the boundaries of odd and even Brillouin zones are found to be

$$\Delta\omega_m = \frac{mqc}{2\sqrt{\epsilon'}} \begin{cases} \left|\rho_m\gamma + \frac{S_m}{8}\gamma^3\right| + \frac{|\rho_m|}{8}\gamma^3, & \text{for odd } m \\ \frac{m}{2}\gamma^2\left|\sum_p \frac{\rho_p\rho_{m-p}}{p}\right|, & \text{for even } m. \end{cases} \quad (12)$$

Using these expressions, the gaps $\Delta\omega_m$ for the model of an SL with arbitrary boundary thickness described by Eq. (1) are plotted as functions of d/l in Fig. 3a for odd gaps and in Fig. 3b for even gaps. In both figures, the gap widths are normalized to the width of the first band gap for an SL with a sinusoidal profile, $\Delta\omega_{1\,\mathrm{sine}}$. The expressions for the widths of odd gaps obtained previously in [26] correspond to the term proportional to γ in Eq. (12) for odd m. In [26], expressions and plots are obtained for gap widths in the spectrum of spin waves; the corresponding dependences for electromagnetic waves can be obtained from them with the following substitution: $\nu = (\omega/c)^2\epsilon_e$ and $\epsilon = \gamma(\omega/c)^2\epsilon_e$ [in the notation of [26], ϵ_e is the permittivity and ϵ is the coefficient (having the dimension of the wave number) of the function $\rho(z)$ in the wave equation]. For the odd Brillouin zones, the dependences of $\Delta\omega_m$ on d/l obtained in [26] (see also [31]) and in this study are qualitatively similar; namely, $\Delta\omega_m$ is virtually independent of d/l for $m = 1$ and rapidly decreases with increasing d/l for $m > 1$. A quantitative difference, related to the inclusion of the terms of third order in γ for odd gaps, is manifested as d/l approaches 1/4; in this case, the term proportional to γ in Eq. (12) tends to zero and for $d/l = 1/4$ the terms that remain in Eq. (12) for odd m describe $\Delta\omega_m$ for odd gaps of a sinusoidal SL. Another difference is related to the appearance of a dip on the $\Delta\omega_m(d)$ plots for odd gaps (for $m = 3$, the dip is close to $d/l = 1/4$; for $m = 5$ and 7, the dip is not seen in the scale chosen).

The dependences of $\Delta\omega_m$ on d/l for even gaps (the lower line in Eq. (12)) are obtained in this study for the first time. In Fig. 3b, we see that the gap $\Delta\omega_m$ is virtually independent of d/l for $m = 2$ and decreases rapidly with increasing d/l for $m > 2$. For an SL with a rectangular profile, $\Delta\omega_m$ for even gaps increases linearly with m. We recall that the expressions obtained remain valid only for those m for which the condition $m\gamma/2 \ll 1$ is satisfied. Therefore, for SLs with $d/l = 0$, the theory developed here is valid only for the values of m for which the widths of even gaps remain smaller than the widths of odd gaps.

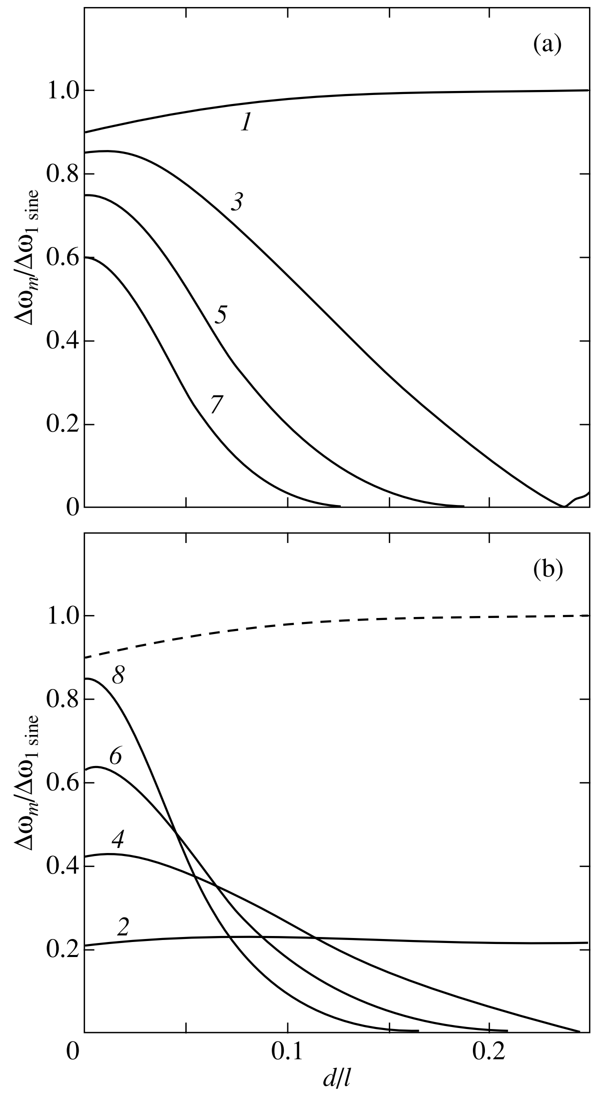

Fig. 3. Dependences of the gap widths $\Delta\omega_m$ at the edge of the mth Brillouin zone on d/l for (a) odd and (b) even gaps for $\gamma = 0.15$. The values of m are indicated on the corresponding curves. The dashed line in panel (b) shows the gap width for the first zone.

3. WAVE DISPERSION LAW

We study the wave dispersion laws in an SL with an arbitrary boundary thickness in the general form for electromagnetic, elastic, and spin waves simultaneously. Such an approach is possible, since the form of the dispersion laws is determined above all by the structure of the SL and its boundary. In this approach, the SL is characterized by a periodic z dependence of a material parameter $A(z)$, which is different for waves of different nature. For example, this parameter can be the permittivity for electromagnetic waves, the density of the material or a force constant for elastic waves, or the magnetization, anisotropy, or exchange constant for spin waves. By analogy with Eq. (2), we write $A(z)$ as

$$A(z) = A[1-\gamma\rho(z)], \tag{13}$$

where A and γ are the static component and the relative root-mean-square modulation of this parameter (the imaginary part of $A(z)$ is disregarded).

We write the wave equation in the form

$$\frac{d^2\mu}{dz^2} + [\nu - \eta\rho(z)]\mu = 0, \tag{14}$$

where the function μ and the parameters ν and η are expressed differently for electromagnetic, elastic, and spin waves. Thus, for spin waves, $\nu = (\omega - \omega_0)/\alpha gM$, where ω_0 is the ferromagnetic resonance frequency, α is the exchange parameter, g is the gyromagnetic ratio, and M is an external magnetic field; for electromagnetic and elastic waves, we have $\nu \propto \omega^2$, etc. (see [26]).

According to the Floquet theorem, the solution to Eq. (14) for waves propagating along the z axis can be represented in the form

$$\mu(z) = e^{-ikz}\sum_{n=-\infty}^{\infty}\mu_n e^{inqz}. \tag{15}$$

Substituting this expression and the Fourier expansion of the function $\rho(z)$ into Eq. (14), we obtain an infinite system of equations for the Fourier transforms μ_n and ρ_n:

$$(\nu - \nu_n)\mu_n = \eta\sum_{n_1}\mu_{n_1}\rho_{n-n_1}, \tag{16}$$

where $\nu = (k - nq)^2$. The dispersion law $\nu = \nu(k)$ can be obtained by equating to zero the determinant of system (16), which contains an infinite number of rows and columns. Numerical analysis of $N \times N$ determinants with finite numbers of rows and columns N allows us to study the wave dispersion law approximately.

However, in many cases, it is more convenient to derive an equation for $\nu(k)$ by expanding into a series in η. This series can be obtained in different ways. We suggest yet another way, where the presence of certain terms in the sums is explicitly forbidden. This approach will be used below when analyzing the effect of such exclusion on the form of the dispersion equation. For generality, we provisionally omit the restriction $\langle\rho(z)\rangle = 0$ used in this study. The quantity ρ_{n-n_1}, which appears on the right-hand side of Eq. (16), can be written in the form

$$\rho_{n-n_1} = \rho_{n-n_1}\delta_{nn_1} + \rho_{n-n_1}\big|_{n_1\neq n}. \tag{17}$$

After substituting Eq. (17) into Eq. (16), we obtain

$$(\nu - \tilde{\nu}_n)\mu_n = \eta\sum_{n_1\neq n}\mu_{n_1}\rho_{n-n_1}, \tag{18}$$

where $\tilde{\nu}_n = \nu_n + \eta\rho_0$. Increasing the index of n_i in Eq. (18) by 1, we express μ_{n_1} from the obtained equation and substitute the result into the right-hand side of Eq. (18). Thus, we obtain

$$(\nu - \tilde{\nu}_n)\mu_n = \eta^2\sum_{n_1\neq n}\sum_{n_2\neq n_1}\frac{\rho_{n-n_1}\rho_{n_1-n_2}\mu_{n_2}}{\nu - \tilde{\nu}_{n_1}}. \tag{19}$$

We represent the product $\rho_{n-n_1}\rho_{n_1-n_2}$ in a form similar to that of Eq. (17),

$$\rho_{n-n_1}\rho_{n_1-n_2} = \rho_{n-n_1}\rho_{n_1-n_2}\delta_{nn_2} + \rho_{n-n_1}\rho_{n_1-n_2}\big|_{n_2\neq n}, \tag{20}$$

and substitute it into Eq. (19), which assumes the form

$$\begin{aligned}&\left(\nu - \tilde{\nu}_n - \eta^2\sum_{n_1\neq n}\frac{\rho_{n-n_1}\rho_{n_1-n}}{\nu - \tilde{\nu}_{n_1}}\right)\mu_n\\ &= \eta^2\sum_{n_1\neq n}\sum_{\substack{n_2\neq n\\ n_2\neq n_1}}\frac{\rho_{n-n_1}\rho_{n_1-n_2}\mu_{n_2}}{\nu - \tilde{\nu}_{n_1}}.\end{aligned} \tag{21}$$

Next, we increase the index of n_i in Eq. (18) by 2, express μ_{n_2} from the obtained equation, substitute the result into the right-hand side of Eq. (21), and represent the product of the three functions ρ_i in a form analogous to Eq. (20). Continuing this process and using the condition $\mu_n \neq 0$, we obtain the equation

$$\begin{aligned}&\nu - \tilde{\nu}_n - \eta^2\sum_{n_1\neq n}\frac{\rho_{n-n_1}\rho_{n_1-n}}{\nu - \tilde{\nu}_{n_1}}\\ &-\eta^3\sum_{n_1\neq n}\sum_{\substack{n_2\neq n\\ n_2\neq n_1}}\frac{\rho_{n-n_1}\rho_{n_1-n_2}\rho_{n_2-n}}{(\nu - \tilde{\nu}_{n_1})(\nu - \tilde{\nu}_{n_2})} - \ldots = 0.\end{aligned} \tag{22}$$

In [32], this equation was derived using a different method. However, that derivation was somewhat inaccurate, since the exclusion of the terms $n_i \neq n_{i-1}$ in the sums was disregarded.

Next, we apply the original idea of the authors of [32], who represented a series similar to Eq. (22) in a form corresponding to the dispersion equation in the weak-coupling approximation. In our notation, this representation for the main branch has the form

$$(\nu - \tilde{\nu}_0 - \tilde{T}^{(0)})(\nu - \tilde{\nu}_m - T^{(0)}) = T^{(-m)}T^{(m)}, \tag{23}$$

where $T^{(m)}$, $T^{(-m)}$, $T^{(0)}$, and $\tilde{T}^{(0)}$ are series containing no resonant factors. By taking into account all the exclusions $n_i \neq n_{i-1}$, these series can be written as

$$\begin{gathered}
T^{(-m)} = \eta\rho_{-m} + \eta^2 \sum_{n_1 \neq 0, m} \frac{\rho_{-n_1}\rho_{n_1-m}}{\nu - \tilde{\nu}_{n_1}} \\
+ \eta^3 \sum_{n_1 \neq 0, m} \sum_{\substack{n_2 \neq 0, m \\ n_2 \neq n_1}} \frac{\rho_{-n_1}\rho_{n_1-n_2}\rho_{n_2-m}}{(\nu - \tilde{\nu}_{n_1})(\nu - \tilde{\nu}_{n_2})} + \dots, \\
T^{(m)} = \eta\rho_m + \eta^2 \sum_{n_1 \neq 0, m} \frac{\rho_{m-n_1}\rho_{n_1}}{\nu - \tilde{\nu}_{n_1}} \\
+ \eta^3 \sum_{n_1 \neq 0, m} \sum_{\substack{n_2 \neq 0, m \\ n_2 \neq n_1}} \frac{\rho_{m-n_1}\rho_{n_1-n_2}\rho_{n_2}}{(\nu - \tilde{\nu}_{n_1})(\nu - \tilde{\nu}_{n_2})} + \dots, \\
T^{(0)} = \eta^2 \sum_{n_1 \neq 0, m} \frac{\rho_{m-n_1}\rho_{n_1-m}}{\nu - \tilde{\nu}_{n_1}} \\
+ \eta^3 \sum_{n_1 \neq 0, m} \sum_{\substack{n_2 \neq 0, m \\ n_2 \neq n_1}} \frac{\rho_{m-n_1}\rho_{n_1-n_2}\rho_{n_2-m}}{(\nu - \tilde{\nu}_{n_1})(\nu - \tilde{\nu}_{n_2})} + \dots, \\
\tilde{T}^{(0)} = \eta^2 \sum_{n_1 \neq 0, m} \frac{\rho_{-n_1}\rho_{n_1}}{\nu - \tilde{\nu}_{n_1}} \\
+ \eta^3 \sum_{n_1 \neq 0, m} \sum_{\substack{n_2 \neq 0, m \\ n_2 \neq n_1}} \frac{\rho_{-n_1}\rho_{n_1-n_2}\rho_{n_2}}{(\nu - \tilde{\nu}_{n_1})(\nu - \tilde{\nu}_{n_2})} + \dots.
\end{gathered} \tag{24}$$

Equations for the boundaries of the band gaps are obtained by setting $k = mq/2$ in Eq. (23) and have the form

$$\nu = \tilde{\nu}_0 + \frac{\tilde{T}^{(0)} + T^{(0)}}{2} \pm \sqrt{\frac{(\tilde{T}^{(0)} - T^{(0)})^2}{4} + T^{(-m)}T^{(m)}}. \tag{25}$$

Expressions (23)–(25) differ from the corresponding expressions in [32] (in particular, in this study, we have $T^{(-m)} \neq T^{(m)*}$). However, for the case $\langle\rho(z)\rangle = 0$, where exclusions of the form $n_i \neq n_{i-1}$ become unnecessary, the expressions in [32] and our equations (22)–(25) assume the same form. In this case, Eq. (25) takes the form

$$\nu = \nu_0 + T^{(0)} \pm |T^{(-m)}|. \tag{26}$$

By solving Eq. (26) to within terms of the order of η^2, we obtain expressions for the gap boundaries,

$$\nu_m^{\pm} = \nu_0 + \eta^2 \sum_{n_1} \frac{|\rho_{n_1}|^2}{\nu_0 - \nu_{n_1}} \pm \left| \eta\rho_m + \eta^2 \sum_{n_1} \frac{\rho_{n_1}\rho_{m-n_1}}{\nu_0 - \nu_{n_1}} \right| \tag{27}$$

and for the gap widths,

$$\Delta\nu_m = 2\left| \eta\rho_m + \eta^2 \sum_{n_1} \frac{\rho_{n_1}\rho_{m-n_1}}{\nu_0 - \nu_{n_1}} \right|. \tag{28}$$

Just as in Section 2, we consider functions $\rho(z)$ with symmetry of the third kind. With such a function, we seek a solution to Eq. (26) to within terms of the order of η^3 and obtain expressions for $\nu_m^{\pm}$,

$$\begin{gathered}
\nu_m^{\pm} = \nu_0 + \eta^2 \sum_{n_1} \frac{|\rho_{n_1}|^2}{\nu_0 - \nu_{n_1}} \pm \eta^3 |\rho_m| \sum_{n_1} \frac{|\rho_{n_1}|^2}{(\nu_0 - \nu_{n_1})^2} \\
\pm \left| \eta\rho_m + \eta^3 \sum_{n_1, n_2} \frac{\rho_{n_1}\rho_{n_2-n_1}\rho_{m-n_2}}{(\nu_0 - \nu_{n_1})(\nu_0 - \nu_{n_2})} \right|, \\
\text{for odd } m, \\
\nu_m^{\pm} = \nu_0 + \eta^2 \left(\sum_{n_1} \frac{|\rho_{n_1}|^2}{\nu_0 - \nu_{n_1}} \pm \left| \sum_{n_1} \frac{\rho_{n_1}\rho_{m-n_1}}{\nu_0 - \nu_{n_1}} \right| \right), \\
\text{for even } m,
\end{gathered} \tag{29}$$

and for $\Delta\nu_m$,

$$\Delta\nu_m = \begin{cases} \left| 2\eta\rho_m + 2\eta^3 \sum_{n_1, n_2} \frac{\rho_{n_1}\rho_{n_2-n_1}\rho_{m-n_2}}{(\nu_0 - \nu_{n_1})(\nu_0 - \nu_{n_2})} \right| \\ -2\eta^3 |\rho_m| \sum_{n_1} \frac{|\rho_{n_1}|^2}{(\nu_0 - \nu_{n_1})^2}, \\ \text{for odd } m, \\ 2\eta^2 \left| \sum_{n_1} \frac{\rho_{n_1}\rho_{m-n_1}}{\nu_0 - \nu_{n_1}} \right|, \quad \text{for even } m. \end{cases} \tag{30}$$

These expressions describe the gaps in the spectrum of spin waves. For electromagnetic waves, using Eq. (2) for the permittivity ($\epsilon \equiv \epsilon'$, $\epsilon'' = 0$), from Eq. (29) we obtain an expression for $\omega_m^{\pm}$ to within terms of the order of γ^3:

$$\omega_m^{\pm} = \frac{mqc}{2\sqrt{\epsilon}}\begin{cases} 1 \pm \left|\frac{\rho_m}{2}\gamma \pm \frac{|\rho_m|\rho_m}{2}\gamma^2 + \left(\frac{m^2\rho_m}{8}S_1 + \frac{m^4}{32}S_3 + \frac{|\rho_m|^2\rho_m}{2}\right)\gamma^3\right| \\ + \left(\frac{m^2}{32}S_1 - \frac{|\rho_m|^2}{8}\right)\gamma^2 \pm \left(\frac{3m^2|\rho_m|}{16}S_1 - \frac{m^4|\rho_m|}{32}S_2 - \frac{3|\rho_m|^3}{16}\right)\gamma^3, \\ \text{for odd } m \\ 1 + \left(\frac{m^2}{8}\sum_{n_1}\frac{|\rho_{n_1}|^2}{n_1(m-n_1)} \pm \frac{m}{4}\left|\sum_{n_1}\frac{\rho_{n_1}\rho_{m-n_1}}{n_1}\right|\right)\gamma^2, \quad \text{for even } m, \end{cases} \tag{31}$$

where

$$S_1 = \sum_{n_1}\frac{|\rho_{n_1}|^2}{n_1(m-n_1)}, \quad S_2 = \sum_{n_1}\frac{|\rho_{n_1}|^2}{n_1^2(m-n_1)},$$
$$S_3 = \sum_{n_1, n_2}\frac{\rho_{n_1}\rho_{n_2-n_1}\rho_{m-n_2}}{n_1(m-n_1)n_2(m-n_2)}. \tag{32}$$

Generally, it is not easy to determine the widths of odd gaps from Eq. (31), since in the uppermost line of this equation the modulus is taken from an expression that has a variable sign. Therefore, we write out expressions for the gap widths with an accuracy of γ^2;

$$\Delta\omega_m = \frac{mqc}{2\sqrt{\epsilon}}\begin{cases} |\rho_m|\gamma, \quad \text{for odd } m, \\ \frac{m}{2}\gamma^2\left|\sum_{n_1}\frac{\rho_{n_1}\rho_{m-n_1}}{n_1}\right|, \quad \text{for even } m. \end{cases} \tag{33}$$

Let us compare formula (11) for the boundaries of the band gaps $\omega_m^{\pm}$ obtained by the MCMT method with an analogous formula (31) obtained from the exact dispersion equation. We see that the coefficients of the corresponding powers of γ in these formulas are described by substantially different expressions (except for the coefficients of the first power of γ, which coincide). It should be emphasized that the expressions for these coefficients in Eq. (31) are exact, since they were obtained, using perturbation theory, from the exact dispersion equation (22) (or from Eq. (26), which is equivalent to it). Therefore, the difference in the corresponding coefficients between Eq. (31) and Eq. (11) characterizes the accuracy of the MCMT method. In order to get a clear idea about this accuracy, we consider Eqs. (31) and (11) for two limiting cases of boundary thickness: $d/l = 0$ (a rectangular profile) and $d/l = 1/4$ (a sinusoidal profile). For a rectangular profile, the expressions for $\omega_m^{\pm}$ obtained by the MCMT method coincide with the corresponding expressions from perturbation theory, at least up to terms of the order of γ^2, and have the form

$$\omega_m^{\pm} = qc/2\sqrt{\epsilon}\begin{cases} m \pm \frac{\gamma}{\pi} + \frac{\gamma^2}{8}m \pm \ldots, \quad \text{for odd } m \\ m + (1 \pm 2)\frac{\gamma^2}{8}m + \ldots, \text{ for even } m. \end{cases} \tag{34}$$

For a sinusoidal profile, the expressions for $\omega_m^{\pm}$ obtained by the MCMT method differ from the corresponding results of perturbation theory. It appears that the difference between the results obtained by the MCMT method and the results of perturbation theory are greater for the positions of the band gaps than for their widths. Thus, for the boundary frequencies of the first Brillouin zone, we have

$$\omega_1^{\pm} = qc/2\sqrt{\epsilon}\left\{1 \pm \frac{\sqrt{2}}{4}\gamma + \begin{cases} \frac{5}{32}\gamma^2 \pm \frac{19\sqrt{2}}{2^9}\gamma^3 + \ldots, \\ \frac{4}{32}\gamma^2 \pm \frac{20\sqrt{2}}{2^9}\gamma^3 + \ldots, \end{cases}\right. \tag{35}$$

where the lower line corresponds to the MCMT method and the upper line to perturbation theory.

To plot the band gap width as a function of the interface thickness d, we used Eqs. (30) and (31), into which we substituted ρ_m corresponding to the Fourier harmonics of the elliptic sine in Eq. (1). For $\gamma = 0.15$, the $\Delta\omega_m(d/l)$ curves for both odd and even gaps differ only slightly from the corresponding curves in Fig. 3, which were obtained by the MCMT method in the previous section (in the chosen scale, the corresponding curves coincide). The d dependences of $\Delta\nu_m$ for spin waves are plotted in Fig. 4a for odd gaps and in Fig. 4b for even gaps. In both figures, the gap widths are normalized to the width of the first band gap of the SL with a sinusoidal profile, $\Delta\nu_{1\text{sine}}$. The $\Delta\nu_m(d)$ and $\Delta\omega_m(d)$ dependences are qualitatively similar; namely, the gap widths are virtually independent of d for $m = 1$ and 2 and rapidly decrease with increasing d for $m > 2$. For odd gaps, both the $\Delta\nu_m(d)$ and $\Delta\omega_m(d)$ curves exhibit dips, which are not seen in the scale of Fig. 4a. By comparing Figs. 3 and 4, we see that, for electromagnetic and spin waves, the dependences of the gap width on the gap number m are qualitatively different; the difference is most clearly seen for a rectangular modulation profile. For $d/l = 0$, the width of odd gaps for electromagnetic (and, accordingly, elastic) waves depends only weakly on m (Fig. 3a). The width of odd gaps for spin waves decreases rapidly with increasing m (in proportion to $1/m$ if we neglect the effects of the order of η^3; see Fig. 4a). The differences between the m dependences for even gaps are even more substantial. While $\Delta\nu_m$ for spin waves decreases as $1/m$ with increasing m (Fig. 4b), $\Delta\omega_m$ for electromagnetic waves grows in proportion to m (Fig. 3b).

4. CONCLUSIONS

Thus, we have considered wave propagation in one-dimensional superlattices (multilayer structures) with arbitrary thickness of the interlayer boundaries in the structures. To describe the superlattice (SL), we have used a model suggested earlier in [26], in which the modulation profile of a material parameter along the SL axis is described by a Jacobian elliptic sine. The MCMT method was used to study the frequency dependences of the transmittance $D(\omega)$ and reflectance $R(\omega)$ for electromagnetic waves in such an SL. Perturbation theory was used to study the $\omega(k)$ dispersion relations for electromagnetic, elastic, and spin waves in SLs with modulation of the corresponding material parameter (dielectric constant, density of the material, or magnetic anisotropy). The experimental situation where traveling waves are studied corresponds to measurement of the reflectance $R(\omega)$ (or the transmittance $D(\omega)$). With standing waves in any resonator (for example, in the case of spin-wave resonance in a thin magnetic film), the $\omega(k)$ dispersion relation is studied. In both cases, the measured $R(\omega)$ and $\omega(k)$ dependences reveal common features (namely, the frequencies of the gap boundary positions $\omega_m^{\pm}$). In the $\omega(k)$ dispersion law, these frequencies are observed directly, whereas the $R(\omega)$ dependence reveals them as the boundary frequencies of the Bragg mirrors. The analytical expressions obtained for $\omega_m^{\pm}$ by different methods from the $R(\omega)$ and $\omega(k)$ dependences turned out to be substantially different. Since the coefficients of the powers of η found from the $\omega(k)$ dispersion relation are exact, their comparison with the corresponding coefficients of the series in η obtained from the $R(\omega)$ dependence using the MCMT method allowed us to estimate the accuracy of the method. The gap widths were determined by this method with a substantially higher accuracy than the gap positions. The high accuracy of the MCMT method was also noted in [33], where the results obtained by using this method were compared with the results of numerical solution of the wave equation.

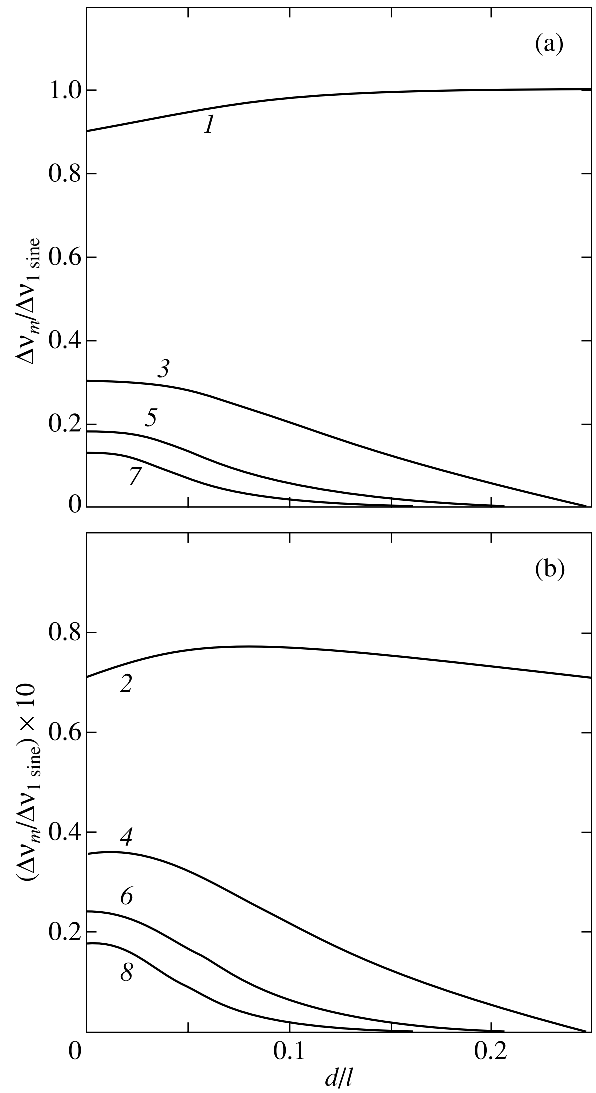

Fig. 4. Dependences of the gap widths $\Delta\nu_m$ at the edge of the mth Brillouin zone on d/l for (a) odd and (b) even gaps for $\eta/q^2 = 0.1$. The values of m are indicated on the corresponding curves. Note that the ordinate scales in panels (a) and (b) are different.

The dependences of the band gap widths $\Delta\omega_m$ and the gap positions in the spectrum on the boundary thickness d have been calculated using both the frequency dependence of the reflectance $R(\omega)$ and the dispersion law. The calculations were performed for both odd and even Brillouin zones of the SL (in a first approximation of perturbation theory, an analogous calculation for odd gaps was performed for the first time in [26]). The dependences of the band gap widths on the gap number for electromagnetic (or elastic) waves ($\Delta\omega_m$) and for spin waves ($\Delta\nu_m$) are different in character. In the case of $d = 0$, for odd gaps, $\Delta\omega_m$ depends only weakly on m, whereas $\Delta\nu_m \propto 1/m$; for even gaps, we have $\Delta\omega_m \propto m$, whereas $\Delta\nu_m \propto 1/m$. The d dependences of the band gap widths are similar in character; namely, the band gap widths for the first and second Brillouin zones are virtually independent of d and the widths of all gaps with $m > 2$ have a strong d dependence. We found a dip in the dependences of $\Delta\omega_m$ and $\Delta\nu_m$ on d/l for $m = 3$, 5, and 7, when higher order terms of perturbation theory were taken into account. The obtained results theoretically substantiate possible experimental methods of measuring the boundary thickness in SLs by using spectral methods. In these methods, it is necessary to measure the widths of two band gaps: $\Delta\omega_1$ and, for example, $\Delta\omega_3$. Then, using the plots in Fig. 3 for electromagnetic or elastic waves and the plots in Fig. 4 for spin waves, one can find d/l from the ratio $\Delta\omega_3/\Delta\omega_1$.

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