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Department of Electrical and Computer Engineering, Wayne State University[1]) *(a) and U.S. Army Research Office*[2]) *(b)*

Confined Acoustic Phonons in a Free-Standing Quantum Well and Their Interaction with Electrons

By

N. BANNOV (a), V. MITIN (a), and M. STROSCIO (b)

The Lagrangian of an isotropic continuous medium and Lagrangian formalism are used to consistently derive acoustic eigenmodes, to normalize them, and to determine the acoustic phonons (confined acoustic phonons) in a free-standing quantum well. These phonons may be classified as shear, dilatational, and flexural phonons in accordance with the acoustic terminology for eigenmodes. The Hamiltonians describing interactions of the confined acoustic phonons with electrons in the approximations of the deformation potential and the piezoelectric scattering potential are obtained and analyzed.

1. Introduction

Many new quantum semiconductor structures have been proposed during the last several years; free-standing quantum wells (FSQWs) and wires (FSQWIs) [1] are among such structures. FSQWs and FSQWIs include thin semiconductor slabs and rods which are connected to a semiconductor substrate by the side of the smallest cross-section. Such exotic structures may be manufactured by diverse etching techniques [1]. Ideal FSQWs and FSQWIs represent waveguides for electron waves which have features substantially different from more conventional quantum structures. First of all, such waveguides may have very high potential energy barriers for electrons, so new effects related to hot but quantized electrons are possible. This phonon subsystem will also undergo substantial modification and quantization of the acoustic phonon spectrum should occur. The quantization of the phonon spectrum has an effect on the electron transport properties and was observed recently [2, 3] in experiments with AuPd quantum wells and quantum wires. To describe quantitatively electron transport peculiarities and predict transport coefficients it is necessary to know all acoustic phonon modes, their spectrum, and their interaction with electrons. The detailed understanding of the confined acoustic phonons in a FSQW and their spectrum may be also significant for some of the nondestructive methods of diagnostic of microstructures where propagation of the acoustic phonons is employed [4 to 6].

While there is an extensive literature on acoustic modes in acoustic waveguides, resonators, and related structures [7, 8], there are relatively few works considering this problem in a context of nanoscale structures [9 to 19]. In [10 to 12, 14, 15] acoustic modes in systems with two interfaces are investigated and attention is drawn primarily to the modes localized between the interfaces. The peculiarities of acoustic phonon modes due to a planar defect have also been considered [18, 19]. It is swhon that a few monolayers of different material

[1]) Detroit, MI-48202, USA.
[2]) P.O. Box 12211, Research Triangle Park, NC-27709-2211, USA.

[19] or even a built-in electron sheet, interacting with phonons through the deformation potential [18] may result in the localization of some acoustic modes on the planar defect. Papers [16, 17] are devoted to one-dimensional acoustic phonons in cylindrical quantum wires.

In this paper we will consider acoustic modes in FSQWs. This problem may be solved exactly if we neglect the distortion of acoustic vibrations resulting from the contact with the semiconductor substrate. This imposes restrictions on the in-plane wavelength, which should be shorter than a characteristic in-plane size of the semiconductor slab. Then we will introduce acoustic phonons for a FSQW and derive the phonon Hamiltonian as well as the Hamiltonian of the electron–phonon interactions. Finally, we discuss the peculiarities of electron scattering from confined acoustic phonons.

2. Formulation of the Problem

Small elastic vibrations of a semiconductor slab can be described by a vector of relative displacement $\boldsymbol{u} = \boldsymbol{u}(\boldsymbol{r}, t)$. The Lagrangian L of an isotropic continuous medium can be expressed in terms of vibrations as (see, for example, [20])

$$L = \tfrac{1}{2} \int [\varrho \dot{\boldsymbol{u}}^2 - \lambda u_{i,i}^2 - 2\mu u_{i,k}^2] \, \mathrm{d}\boldsymbol{r} \,, \tag{1}$$

where ϱ is the density of the semiconductor, λ, μ are the Lamé constants, $u_{i,j}$ is the strain tensor,

$$u_{i,j} = \frac{1}{2} \left(\frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i} \right),$$

and a dot over $\boldsymbol{u}$ denotes differentiation with respect to time. The sum is assumed to be taken over repeated Roman subscripts. The equations of motion of elastic continua described by (1) follow from the principle of the least action and have the form

$$\varrho \frac{\partial^2 u_\alpha}{\partial t^2} = \frac{\partial \sigma_{\alpha,j}}{\partial r_j}, \tag{2}$$

where $\sigma_{i,j}$ is the stress tensor

$$\sigma_{i,j} = \lambda u_{k,k} \delta_{i,j} + 2\mu u_{i,j} \,,$$

$\delta_{i,j}$ ist the Kronecker delta. Equation (2) can be rewritten in a vector form as

$$\frac{\partial^2 \boldsymbol{u}}{\partial t^2} = s_\mathrm{t}^2 \nabla^2 \boldsymbol{u} + (s_\mathrm{l}^2 - s_\mathrm{t}^2) \, \mathrm{grad} \, \mathrm{div} \, \boldsymbol{u} \,, \tag{3}$$

where $s_\mathrm{l} = (\lambda + 2\mu)/\varrho$ and $s_\mathrm{t} = \mu/\varrho$ are the velocities of longitudinal and transverse acoustic waves in bulk semiconductors. The boundary conditions on the free surface of the slab imply that the components of the stress tensor corresponding to the normal direction to the surface vanish. If we specify the coordinate system (which we will use throughout this paper) in such a way that the z-axis is perpendicular to the semiconductor slab and the surfaces of the slab have coordinates $z = \pm (a/2)$, where a is the width of the slab, the boundary conditions take the form $\sigma_{x,z} = \sigma_{y,z} = \sigma_{z,z} = 0$ at $z = \pm (a/2)$; accordingly in

terms of the components of the displacement vector, it follows that

$$\sigma_{x,z} = \mu\left(\frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x}\right) = 0\,,$$

$$\sigma_{y,z} = \mu\left(\frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y}\right) = 0\,, \tag{4}$$

$$\sigma_{z,z} = \lambda\,\mathrm{div}\,\boldsymbol{u} + 2\mu\,\frac{\partial u_z}{\partial z} = 0$$

at $z = \pm(a/2)$. Our goal is to find the eigenmodes of the acoustic vibrations defined by (3) and (4). We will look for solutions in the following form:

$$\boldsymbol{u}(\boldsymbol{r}, t) = \sum_n \int \boldsymbol{u}_n(\boldsymbol{q}_\parallel, z)\exp\left(i\boldsymbol{q}_\parallel \boldsymbol{r}_\parallel - i\omega_n t\right)\frac{\mathrm{d}\boldsymbol{q}_\parallel}{(2\pi)^2}\,, \tag{5}$$

where $\boldsymbol{r}_\parallel$ is the coordinate vector in the (x, y) plane, ω_n is the set of frequencies of vibrations. From (3) we can obtain the set of equations for eigenmodes, $\boldsymbol{u}_n(\boldsymbol{q}_\parallel, z)$, and eigenfrequencies, ω_n. This may be conveniently done if we direct the x-axis of the coordinate system along the vector $\boldsymbol{q}_\parallel$, so that $\boldsymbol{q}_\parallel = (q_x, 0)$. Then the eigenvalue problem takes the form

$$\mathscr{D}\boldsymbol{u}_n(\boldsymbol{q}_\parallel, z) = -\omega_n^2 \boldsymbol{u}_n(\boldsymbol{q}_\parallel, z)\,, \tag{6}$$

where $\mathscr{D}$ is the matrix differential operator,

$$\mathscr{D} = \begin{bmatrix} s_t^2\dfrac{d^2}{dz^2} - s_l^2 q_x^2 & 0 & (s_l^2 - s_t^2)\,iq_x\dfrac{d}{dz} \\ 0 & s_t^2\dfrac{d^2}{dz^2} - s_t^2 q_x^2 & 0 \\ (s_l^2 - s_t^2)\,iq_x\dfrac{d}{dz} & 0 & s_l^2\dfrac{d^2}{dz^2} - s_t^2 q_x^2 \end{bmatrix}. \tag{7}$$

The boundary conditions (4) become

$$\frac{\mathrm{d}u_x}{\mathrm{d}z} = -iq_x u_z\,, \qquad \frac{\mathrm{d}u_y}{\mathrm{d}z} = 0, \qquad \frac{\mathrm{d}u_z}{\mathrm{d}z} = -iq_x\frac{s_l^2 - 2s_t^2}{s_l^2}\,u_x \tag{8}$$

at $z = \pm(a/2)$. It can be proved straightforwardly that the operator $\mathscr{D}$ of the eigenvalue problem (6) to (8) is Hermitian, thus the eigenfunctions, $\boldsymbol{u}_n(\boldsymbol{q}_\parallel, z)$, corresponding to nondegenerate eigenfrequencies, ω_n, are orthogonal. We can also orthogonalize the eigenfunctions corresponding to equal eigenfrequencies using the Schmidt orthogonalization procedure. We will use $\boldsymbol{w}$ instead of $\boldsymbol{u}$ to denote the orthonormal set of eigenvectors, $\boldsymbol{w}_n(\boldsymbol{q}_\parallel, z)$, of the problem (6) to (8) for which

$$\int \boldsymbol{w}_n^\dagger(\boldsymbol{q}_\parallel, z)\,\boldsymbol{w}_m(\boldsymbol{q}_\parallel, z)\,\mathrm{d}z = \delta_{n,m}\,. \tag{9}$$

3. Confined Eigenmodes

The eigenvalue problem (6), (7) can be solved through the introduction of vector and scalar mechanical potentials which define the vector of the relative displacement [7, 8]. In this section we will identify such modes employing the conventional terminology of acoustics

[7, 8]. The major feature of the confined modes is their quantization in the z-direction. Roughly speaking, the z-components of the confined mode wave vectors, q_z, take only some discrete set of values at each particular in-plane wave vector, $\boldsymbol{q}_{\|}$. There are three different types of confined acoustic modes: shear waves, dilatational waves, and flexural waves. They are characterized by their distinctive symmetries.

3.1 Shear waves

These waves have only nonzero component which is perpendicular to the direction of wave propagation and lies in the plane of the quantum well: $\boldsymbol{u}_n(\boldsymbol{q}_{\|}, z) = (0, u_y, 0)$, where

$$u_y = \begin{cases} \cos(q_{z,n} z), & \text{if} \quad n = 0, 2, 4, \ldots, \\ \sin(q_{z,n} z), & \text{if} \quad n = 1, 3, 5, \ldots; \end{cases} \tag{10}$$

$q_{z,n} = (\pi n/a)$. The dispersion relation for shear waves is

$$\omega_n = s_t \sqrt{q_{z,n}^2 + q_x^2}\,.$$

These modes are similar to the transverse modes in bulk semiconductors and their quantization is based on the simple rule stating that an integer number of half wavelengths fits in a semiconductor slab of width a.

3.2 Dilatational waves

These waves are also called symmetric waves (in respect to the midplane) and have two nonzero components: $\boldsymbol{u}_n(\boldsymbol{q}_{\|}, z) = (u_x, 0, u_z)$, where

$$u_x = iq_x \left[(q_x^2 - q_t^2) \sin \frac{q_t a}{2} \cos q_l z + 2q_l q_t \sin \frac{q_l a}{2} \cos q_t z \right], \tag{11}$$

$$u_z = q_l \left[-(q_x^2 - q_t^2) \sin \frac{q_t a}{2} \sin q_l z + 2q_x^2 \sin \frac{q_l a}{2} \sin q_t z \right]. \tag{12}$$

The parameters q_l, q_t are determined from the system of two algebraic equations

$$\frac{\tan(q_t a/2)}{\tan(q_l a/2)} = -\frac{4q_x^2 q_l q_t}{(q_x^2 - q_t^2)^2}, \tag{13}$$

$$s_l^2(q_x^2 + q_l^2) = s_t^2(q_x^2 + q_t^2). \tag{14}$$

Equations (13) and (14) have many solutions for q_l and q_t at each particular q_x [7] and we number them by an additional index n: $q_{l,n}$, $q_{t,n}$. These solutions are either real or pure imaginary depending on q_x and n. Thus, the quantization rule for dilatational waves prescribed by (13) and (14) is nontrivial because these modes represent linear combinations of z-coordinate dependent harmonics. The frequencies of the dilatational waves are given by

$$\omega_n = s_l \sqrt{q_x^2 + q_{l,n}^2} = s_t \sqrt{q_x^2 + q_{t,n}^2}\,. \tag{15}$$

3.3 Flexural waves

The last type of waves in quantum wells are flexural or antisymmetric waves. Flexural waves have two nonzero components $\boldsymbol{u}_n(\boldsymbol{q}_\parallel, z) = (u_x, 0, u_z)$;

$$u_x = iq_x \left[(q_x^2 - q_t^2) \cos \frac{q_t a}{2} \sin q_l z + 2q_l q_t \cos \frac{q_l a}{2} \sin q_t z \right], \tag{16}$$

$$u_z = q_l \left[(q_x^2 - q_t^2) \cos \frac{q_t a}{2} \cos q_l z - 2q_x^2 \cos \frac{q_l a}{2} \cos q_t z \right], \tag{17}$$

where q_l, q_t are determined from the solution of the transcendental equation

$$\frac{\tan (q_l a/2)}{\tan (q_t a/2)} = - \frac{4q_x^2 q_l q_t}{(q_x^2 - q_t^2)^2} \tag{18}$$

and equation (14). The system of algebraic equations (14) and (18) prescribing the quantization rule for flexural waves also has many solutions for q_l and q_t at each particular q_x [7] and we again use an additional index n to number them: $q_{l,n}$, $q_{t,n}$. Solutions q_l and q_t may be either real numbers or pure imaginary numbers for the given set q_x and n. The dispersion relation for flexural waves coincides with the relation for dilatational waves (15) (this does not result in the coincidence of frequencies because the solutions for $q_{l,n}$ and $q_{t,n}$ are different for dilatational and flexural modes).

Now we introduce the normalization constants $F_{s,n}$, $F_{d,n}$, and $F_{f,n}$, such that $\boldsymbol{w}_n = F_{s,n}\boldsymbol{u}_n$ for shear waves, $\boldsymbol{w}_n = F_{d,n}\boldsymbol{u}_n$ for dilatational waves, and $\boldsymbol{w}_n = F_{f,n}\boldsymbol{u}_n$ for flexural waves. The functions $\boldsymbol{u}_n$ are determined by (10) for shear waves, by (11) and (12) for dilatational waves, and by (16) and (17) for flexural waves. The functions $\boldsymbol{w}_n$ satisfy the orthonormality condition (9). The normalization constants $F_{s,n}$, $F_{d,n}$, and $F_{f,n}$ may be determined straightforwardly, however, explicit expressions for these normalization constants are quite cumbersome and, accordingly, we give them in the Appendix.

4. Quantization of Confined Vibrations

The Lagrangian formalism is now used to quantize acoustic phonons. The starting point for the quantization of acoustic vibrations is the commutator

$$[\Pi_\alpha(\boldsymbol{r}, t), u_\beta(\boldsymbol{r}', t)] = -i\hbar\delta_{\alpha,\beta}\, \delta(\boldsymbol{r} - \boldsymbol{r}'), \tag{19}$$

where $\Pi(\boldsymbol{r}, t) = \delta L/\delta\dot{\boldsymbol{u}}(\boldsymbol{r}, t) = \varrho\dot{\boldsymbol{u}}(\boldsymbol{r}, t)$ is the canonical momentum conjugate to the velocity $\dot{\boldsymbol{u}}(\boldsymbol{r}, t)$, and α and β represent the x, y, z components of appropriate vectors. Now we introduce the Fourier transforms of the relative displacement, $\boldsymbol{u}(\boldsymbol{r}, t)$ and velocity, $\dot{\boldsymbol{u}}(\boldsymbol{r}, t)$, in accordance with the formulae

$$\boldsymbol{u}(\boldsymbol{r}, t) = \int \boldsymbol{u}(\boldsymbol{q}_\parallel, z, t) \exp (i\boldsymbol{q}_\parallel \boldsymbol{r}_\parallel) \frac{\mathrm{d}\boldsymbol{q}_\parallel}{(2\pi)^2},$$

$$\dot{\boldsymbol{u}}(\boldsymbol{r}, t) = \int \dot{\boldsymbol{u}}(\boldsymbol{q}_\parallel, z, t) \exp (i\boldsymbol{q}_\parallel \boldsymbol{r}_\parallel) \frac{\mathrm{d}\boldsymbol{q}_\parallel}{(2\pi)^2}.$$

The first term of the Lagrangian (1) corresponding to the kinetic energy may be rewritten as

$$K = \frac{1}{2}\int \varrho \dot{\boldsymbol{u}}^{\dagger}(\boldsymbol{q}_{\|}, z, t)\, \dot{\boldsymbol{u}}(\boldsymbol{q}_{\|}, z, t)\, \mathrm{d}z\, \frac{\mathrm{d}\boldsymbol{q}_{\|}}{(2\pi)^2}\,.$$

The canonical momentum $\boldsymbol{P}(\boldsymbol{q}_{\|}, z, t)$ conjugate to the velocity $\dot{\boldsymbol{u}}(\boldsymbol{q}_{\|}, z, t)$, is defined as

$$\boldsymbol{P}(\boldsymbol{q}_{\|}, z, t) = \frac{\delta L}{\delta \dot{\boldsymbol{u}}(\boldsymbol{q}_{\|}, z, t)} = \frac{\delta K}{\delta \dot{\boldsymbol{u}}(\boldsymbol{q}_{\|}, z, t)} = \frac{\varrho}{(2\pi)^2}\, \dot{\boldsymbol{u}}^{\dagger}(\boldsymbol{q}_{\|}, z, t)\,.$$

The vectors $\boldsymbol{P}(\boldsymbol{q}_{\|}, z, t)$ and $\boldsymbol{u}(\boldsymbol{q}_{\|}, z, t)$ should be treated as operators whose commutational relations may be derived from (19) and have the following form:

$$[P_{\alpha}(\boldsymbol{q}_{\|}, z, t), u_{\beta}(\boldsymbol{q}'_{\|}, z', t)] = -i\hbar\delta_{\alpha,\beta}\, \delta(z - z')\, \delta(\boldsymbol{q}_{\|} - \boldsymbol{q}'_{\|})\,. \tag{20}$$

The Fourier transform, $\boldsymbol{u}(\boldsymbol{q}_{\|}, z, t)$, of the relative displacement vector is a function and an operator which acts on phonon states. We may expand $\boldsymbol{u}(\boldsymbol{q}_{\|}, z, t)$ as a function of z in a series of $\boldsymbol{w}_n(\boldsymbol{q}_{\|}, z)$, which forms a complete set in the space of functions of possible displacements depending on the (x, y) coordinates through the functional form $\exp(i\boldsymbol{k}_{\|}\boldsymbol{r}_{\|})$,

$$\boldsymbol{u}(\boldsymbol{q}_{\|}, z, t) = \sum_n [B_n(\boldsymbol{q}_{\|}, t) + B_n^{\dagger}(-\boldsymbol{q}_{\|}, t)]\, \boldsymbol{w}_n(\boldsymbol{q}_{\|}, z)\,. \tag{21}$$

The coefficient preceding $\boldsymbol{w}_n(\boldsymbol{q}_{\|}, z)$ has been chosen in such a form that the symmetry condition, $\boldsymbol{u}(\boldsymbol{q}_{\|}, z, t) = \boldsymbol{u}^{\dagger}(-\boldsymbol{q}_{\|}, z, t)$, for the Fourier transform of the relative displacement is ensured. The basis functions, $\boldsymbol{w}(\boldsymbol{q}_{\|}, z)$, satisfy the same symmetry condition, $\boldsymbol{w}(\boldsymbol{q}_{\|}, z) = \boldsymbol{w}^{\dagger}(-\boldsymbol{q}_{\|}, z)$, as implied by (6) and (7). The operators $B_n(\boldsymbol{q}_{\|}, t)$ depend on time as $\exp(-i\omega_n t)$, so the momentum, $\boldsymbol{P}(\boldsymbol{q}_{\|}, z, t)$, may be written as

$$\boldsymbol{P}(\boldsymbol{q}_{\|}, z, t) = \frac{\varrho}{(2\pi)^2} \sum_n i\omega_n [B_n^{\dagger}(\boldsymbol{q}_{\|}, t) - B_n(-\boldsymbol{q}_{\|}, t)]\, \boldsymbol{w}_n^{\dagger}(\boldsymbol{q}_{\|}, z)\,. \tag{22}$$

The operators $B_n(\boldsymbol{q}_{\|}, t)$ and $B_n^{\dagger}(\boldsymbol{q}_{\|}, t)$ are expressed in terms of $\boldsymbol{u}(\boldsymbol{q}_{\|}, z, t)$ and $\boldsymbol{P}(\boldsymbol{q}_{\|}, z, t)$ as

$$B_n(\boldsymbol{q}_{\|}, t) = \frac{1}{2}\int \boldsymbol{w}_n^{\dagger}(\boldsymbol{q}_{\|}, z) \left[\boldsymbol{u}(\boldsymbol{q}_{\|}, z, t) + \frac{i}{\omega_n}\frac{(2\pi)^2}{\varrho}\boldsymbol{P}(-\boldsymbol{q}_{\|}, z, t)\right] \mathrm{d}z\,, \tag{23}$$

$$B_n^{\dagger}(\boldsymbol{q}_{\|}, t) = \frac{1}{2}\int \boldsymbol{w}_n(\boldsymbol{q}_{\|}, z) \left[\boldsymbol{u}(-\boldsymbol{q}_{\|}, z, t) - \frac{i}{\omega_n}\frac{(2\pi)^2}{\varrho}\boldsymbol{P}(\boldsymbol{q}_{\|}, z, t)\right] \mathrm{d}z\,. \tag{24}$$

The commutation relations for $B_n(\boldsymbol{q}_{\|}, t)$ and $B_n^{\dagger}(\boldsymbol{q}_{\|}, t)$ follow from (23), (24), and (20),

$$[B_n(\boldsymbol{q}_{\|}, t), B_m^{\dagger}(\boldsymbol{q}'_{\|}, t)] = \frac{2\pi^2\hbar}{\varrho\sqrt{\omega_n\omega_m}}\, \delta_{n,m}\, \delta(\boldsymbol{q}_{\|} - \boldsymbol{q}'_{\|})\,.$$

Now we introduce new operators $b_n(\boldsymbol{q}_{\|}, t)$ and $b_n^{\dagger}(\boldsymbol{q}_{\|}, t)$ in accordance with the definitions

$$B_n(\boldsymbol{q}_{\|}, t) = \sqrt{\frac{\hbar A}{2\varrho\omega_n}}\, b_n(\boldsymbol{q}_{\|}, t)\,, \tag{25}$$

$$B_n^{\dagger}(\boldsymbol{q}_{\|}, t) = \sqrt{\frac{\hbar A}{2\varrho\omega_n}}\, b_n^{\dagger}(\boldsymbol{q}_{\|}, t)\,. \tag{26}$$

The operators $b_n(\boldsymbol{q}_\parallel, t)$ and $b_n^\dagger(\boldsymbol{q}_\parallel, t)$ obey the commutational relations

$$[b_n(\boldsymbol{q}_\parallel, t), b_m^\dagger(\boldsymbol{q}'_\parallel, t)] = \delta_{n,m}\delta_{\boldsymbol{q}_\parallel,\boldsymbol{q}'_\parallel}, \tag{27}$$

in which the variable $\boldsymbol{q}_\parallel$ was redefined in (25) and (26) as a discrete variable. The factor A in (25) and (26) denotes the area of the slab in the (x, y) plane. From the commutator (27) we conclude that $b_n(\boldsymbol{q}_\parallel, t)$ and $b_n^\dagger(\boldsymbol{q}_\parallel, t)$ correspond to the creation and annihilation operators for the confined acoustic phonons, respectively. The phonon Hamiltonian

$$H_{\text{ph}} = \int \boldsymbol{P}(\boldsymbol{q}_\parallel, z, t)\, \dot{\boldsymbol{u}}(\boldsymbol{q}_\parallel, z, t)\, \mathrm{d}\boldsymbol{q}_\parallel\, \mathrm{d}z - L$$

takes the canonical form,

$$H_{\text{ph}} = \sum_n \hbar\omega_n(\boldsymbol{q}_\parallel)\, [b_n^\dagger(\boldsymbol{q}_\parallel, t)\, b_n(\boldsymbol{q}_\parallel, t) + \tfrac{1}{2}], \tag{28}$$

if we replace $\boldsymbol{P}(\boldsymbol{q}_\parallel, z, t)$, $\dot{\boldsymbol{u}}(\boldsymbol{q}_\parallel, z, t)$, and $\boldsymbol{u}(\boldsymbol{q}_\parallel, z, t)$ using (21) and (22) and take into account (25) and (26). All operators considered in this section are time dependent as they are in the Heisenberg representation. We will use $c_n(\boldsymbol{q}_\parallel)$, $c_n^\dagger(\boldsymbol{q}_\parallel)$ to denote creation and annihilation operators in the Schrödinger representation. The Hamiltonian (28) is invariant in respect to the transition between these two representations.

5. Hamiltonian for Electron–Phonon Interactions

The operator for the relative displacement, $\boldsymbol{u}(\boldsymbol{r})$, in the Schrödinger representation in terms of $c_n(\boldsymbol{q}_\parallel)$ and $c_n^\dagger(\boldsymbol{q}_\parallel)$ follows from (21), (25), and (26) and has the form

$$\boldsymbol{u}(\boldsymbol{r}) = \sum_{\boldsymbol{q}_\parallel, n} \sqrt{\frac{\hbar}{2A\varrho\omega_n(\boldsymbol{q}_\parallel)}}\, [c_n(\boldsymbol{q}_\parallel) + c_n^\dagger(-\boldsymbol{q}_\parallel)]\, \boldsymbol{w}_n(\boldsymbol{q}_\parallel, z)\, \mathrm{e}^{i\boldsymbol{q}_\parallel \boldsymbol{r}_\parallel}. \tag{29}$$

5.1 Deformation potential interaction

At first, we will consider the approximation of the deformation potential for the derivation of the Hamiltonian of the electron–phonon interaction (see, for example, [21]),

$$H_{\text{def}} = E_{\text{a}}\, \text{div}\, \boldsymbol{u}(\boldsymbol{r}), \tag{30}$$

where E_{a} is a deformation potential coupling constant. From (29) and (30) it follows that

$$H_{\text{def}} = \sum_{\boldsymbol{q}_\parallel, n} \mathrm{e}^{i\boldsymbol{q}_\parallel \boldsymbol{r}_\parallel}\, \Gamma(\boldsymbol{q}_\parallel, n, z)\, [c_n(\boldsymbol{q}_\parallel) + c_n^\dagger(-\boldsymbol{q}_\parallel)], \tag{31}$$

where

$$\Gamma(\boldsymbol{q}_\parallel, n, z) = \sqrt{\frac{\hbar E_{\text{a}}^2}{2A\varrho\omega_n(\boldsymbol{q}_\parallel)}} \left(i\boldsymbol{q}_\parallel w_n(\boldsymbol{q}_\parallel, z) + \frac{\partial w_{nz}(\boldsymbol{q}_\parallel, z)}{\partial z} \right). \tag{32}$$

It is obvious for shear waves that $\Gamma_{\text{s}}(\boldsymbol{q}_\parallel, n) = 0$. Hence, shear waves do not interact with electrons; this is in line with the fact that transverse phonons in a bulk isotropic solid do not interact with electrons through the deformation potential. On the contrary, both dilatational and flexural waves contribute to the Hamiltonian for electron–acoustic phonon scattering. Accordingly, the functions Γ_{d} and Γ_{f}, describing the intensity of the electron

interactions with dilatational and flexural waves are given by

$$\Gamma_{\mathrm{d}}(\boldsymbol{q}_{\|}, n, z) = F_{\mathrm{d},n} \sqrt{\frac{\hbar E_{\mathrm{a}}^2}{2A\varrho\omega_n(\boldsymbol{q}_{\|})}} \left[(q_{\mathrm{t},n}^2 - q_x^2)\,(q_{\mathrm{l},n}^2 + q_x^2) \sin\left(\frac{aq_{\mathrm{t},n}}{2}\right) \cos\,(q_{\mathrm{l},n} z) \right], \tag{33}$$

$$\Gamma_{\mathrm{f}}(\boldsymbol{q}_{\|}, n, z) = F_{\mathrm{f},n} \sqrt{\frac{\hbar E_{\mathrm{a}}^2}{2A\varrho\omega_n(\boldsymbol{q}_{\|})}} \left[(q_{\mathrm{t},n}^2 - q_x^2)\,(q_{\mathrm{l},n}^2 + q_x^2) \cos\left(\frac{aq_{\mathrm{t},n}}{2}\right) \sin\,(q_{\mathrm{l},n} z) \right]. \tag{34}$$

From (33) and (34) we may see an interesting feature of the functions Γ_{d} and Γ_{f}; they depend on the z-coordinate as functions $\cos(q_{\mathrm{l}}z)$ and $\sin(q_{\mathrm{l}}z)$ (obtained from displacements associated with "longitudinal" vibrations), although the eigenmodes (11), (12), (16), (17) also have $\cos(q_{\mathrm{t}}z)$ and $\sin(q_{\mathrm{t}}z)$ terms which may be associated with "transverse" vibrations; these "transverse" terms were cancelled in the calculation of functions Γ and do not appear in the final results.

Another important property of the functions Γ_{d} and Γ_{f} is their opposite symmetry. The function Γ_{d} is symmetric, but the function Γ_{f} is antisymmetric. This results in substantially different contributions to electron scattering from dilatational and flexural phonons. If the electron potential energy in the FSQW is a symmetric function of z-coordinate, the electron states may be classified by the symmetry of the electron wave function into symmetric and antisymmetric states. Dilatational phonons will interact only with electrons scattered between two states of the same symmetry while the scattering by flexural phonons will result in the electron transition between two states of opposite symmetry.

5.2 Piezoelectric potential interaction

Now we will consider the interaction of acoustic phonons with electrons through the piezoelectric potential. This mechanism of electron–phonon scattering is inherent to crystals without an inversion center, for example, zincblende polar semiconductors. The appropriate Hamiltonian has the form

$$H_{\mathrm{pz}} = -e\varphi(\boldsymbol{r}), \tag{35}$$

where $\varphi(\boldsymbol{r})$ is an electric potential, associated with acoustic waves in the piezoelectric medium. An arbitrary deformation of the piezoelectric semiconductors is accompanied by a polarization vector $\mathscr{P}$ which is related to the strain tensor u_{ij} as

$$\mathscr{P}_v = \beta_{v,ij} u_{ij},$$

where $\beta_{v,ij}$ is a polarization tensor [8]. The electric potential φ may be determined from Poisson's equation, div $\boldsymbol{D} = 0$, where

$$D_i(\boldsymbol{r}) = -\varepsilon_{ij} \frac{\partial\varphi}{\partial r_j} + 4\pi\mathscr{P}_i$$

and ε_{ij} is a low frequency dielectric permittivity tensor. For zincblende semiconductors $\varepsilon_{ij} = \varepsilon\delta_{ij}$, and the piezoelectric tensor has only one independent component $\beta_{x,yz} = \beta_{y,zx} = \beta_{z,xy} = \beta$; $\beta_{v,ij} = 0$, if $v = i$, or $v = j$, or $i = j$ in the Cartesian coordinate system associated with the axes of symmetry of the crystal.

If we adopt the above-mentioned simplifications, Poisson's equation takes the form

$$\nabla^2\varphi = \frac{8\pi\beta}{\varepsilon}\left(\frac{\partial^2 u_x}{\partial y\,\partial z} + \frac{\partial^2 u_y}{\partial z\,\partial x} + \frac{\partial^2 u_z}{\partial x\,\partial y}\right), \tag{36}$$

where the right-hand side is determined by (29). Using the solutions of (36) we may represent the Hamiltonian of the piezoelectric scattering (35) in the following form:

$$H_{pz} = \sum_{\boldsymbol{q}_\parallel, n} e^{i\boldsymbol{q}_\parallel \boldsymbol{r}_\parallel}\, V(\boldsymbol{q}_\parallel, n, z)\,[c_n(\boldsymbol{q}_\parallel) + c_n^\dagger(-\boldsymbol{q}_\parallel)]\,, \tag{37}$$

where the function $V(\boldsymbol{q}_\parallel, n, z)$ is a solution of the ordinary differential equation

$$\begin{aligned}&\frac{\partial^2 V(\boldsymbol{q}_\parallel, n, z)}{\partial z^2} - \boldsymbol{q}_\parallel^2 V(\boldsymbol{q}_\parallel, n, z)\\ &= -\mathscr{B}_n(\boldsymbol{q}_\parallel)\left(iq_y\frac{\partial w_{nx}(\boldsymbol{q}_\parallel, z)}{\partial z} + iq_x\frac{\partial w_{ny}(\boldsymbol{q}_\parallel, z)}{\partial z} - q_x q_y w_{nz}(\boldsymbol{q}_\parallel, z)\right);\end{aligned} \tag{38}$$

$$\mathscr{B}_n(\boldsymbol{q}_\parallel) = \frac{8\pi e\beta}{\varepsilon}\sqrt{\frac{\hbar}{2A\varrho\omega_n(\boldsymbol{q}_\parallel)}}\,.$$

Unlike the deformation potential Hamiltonian of (31) and (32), the Hamiltonian of the piezoelectric scattering, defined by (37) and (38) couples electrons with all three types of acoustic phonons in the semiconductor slab — shear waves, dilatational waves, and flexural waves. Moreover, H_{pz} is anisotropic due to the anisotropy of the polarization tensor $\beta_{v,ij}$. The coupling functions for shear phonons, $V_s(\boldsymbol{q}_\parallel, n, z)$, dilatational phonons, $V_d(\boldsymbol{q}_\parallel, n, z)$ and flexural phonons, $V_f(\boldsymbol{q}_\parallel, n, z)$, obtained by solving (38) have the following forms:

$$V_s(\boldsymbol{q}_\parallel, n, z) = iF_{s,n}\mathscr{B}_n(\boldsymbol{q}_\parallel)\frac{(q_x^2 - q_y^2)(\pi n/a)}{(\boldsymbol{q}_\parallel^2 + (\pi n/a)^2)\,\boldsymbol{q}_\parallel}\begin{cases} -\sin\left(\dfrac{\pi n z}{a}\right), & \text{if} \quad n = 0, 2, 4, \dots,\\ \cos\left(\dfrac{\pi n z}{a}\right), & \text{if} \quad n = 1, 3, 5, \dots,\end{cases} \tag{39}$$

$$V_d(\boldsymbol{q}_\parallel, n, z) = F_{d,n}\mathscr{B}_n(\boldsymbol{q}_\parallel)\,q_x q_y q_l \times\left[\frac{3(q_\parallel^2 - q_t^2)}{q_\parallel^2 + q_l^2}\sin\left(\frac{q_l a}{2}\right)\sin(q_l z) - \frac{2(q_\parallel^2 - 2q_t^2)}{q_\parallel^2 + q_t^2}\sin\left(\frac{q_l a}{2}\right)\sin(q_t z)\right], \tag{40}$$

$$V_f(\boldsymbol{q}_\parallel, n, z) = -F_{f,n}\mathscr{B}_n(\boldsymbol{q}_\parallel)\,q_x q_y q_l \times\left[\frac{3(q_\parallel^2 - q_t^2)}{q_\parallel^2 + q_l^2}\cos\left(\frac{q_l a}{2}\right)\cos(q_l z) - \frac{2(q_\parallel^2 - 2q_t^2)}{q_\parallel^2 + q_t^2}\cos\left(\frac{q_l a}{2}\right)\cos(q_t z)\right]. \tag{41}$$

The functions V_d and V_f have opposite symmetry; the function V_d is antisymmetric and the function V_f is symmetric. The symmetry of the functions V_d and V_f is opposite to the symmetry of the coupling functions Γ_d and Γ_f for deformation potential interaction. Accordingly, if the electron potential energy is symmetric, the dilatational phonons will interact through the piezoelectric potential only with electrons scattered between two states of opposite symmetry and flexural phonons — with electrons scattered between two states of the same symmetry. Another difference between the deformation potential coupling functions Γ_d and Γ_f and the piezoelectric potential coupling functions V_d and V_f is that the

piezoelectric potential coupling functions include terms sin $(q_t z)$ and cos $(q_t z)$ which were absent in the deformation potential coupling functions. The electron–shear phonon coupling function V_s is symmetric for odd modes and antisymmetric for even modes, thus the electron scattering by shear phonons may result in electron transitions between two states of any symmetry.

It is interesting to note that there is a significant similarity between the Hamiltonian for electron interactions with confined acoustic phonons and interactions with confined and interface optical phonons (see, for example, [22]). In both cases electrons interact with many phonon modes and the spatial dependence of the Hamiltonian in the z-direction is a linear combination of either sin and cos functions or sinh and cosh functions (in the case of optical phonons this corresponds to either confined or interface phonons). However, the acoustic phonon energy is a strong function of the quantum number, corresponding to motion transverse to the slab whereas the optical phonon energy dependence on the value of the similar quantum number is weak.

6. Conclusions

We have determined the confined acoustic phonons in a FSQW, corresponding to the shear, dilatational, and flexural acoustic waves in a solid slab. In addition, we have obtained the expression for the relative displacement vector in terms of acoustic phonon amplitudes. The Hamiltonians of the electron–confined phonon interactions through the deformation potential, H_{def}, and the piezoelectric potential, H_{pz}, are derived. It is shown that H_{def} couples electrons only with dilatational and flexural acoustic waves, while H_{pz} is responsible for electron interactions with all three types of phonons.

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Appendix

In this appendix we present formulae for the normalization constants $F_{s,n}$, $F_{d,n}$, and $F_{f,n}$ for shear waves, dilatational waves, and flexural waves. To make the formulae more concise, we omit the index n when specifying $q_{l,n}$ and $q_{t,n}$, because this will not cause confusion. These formulae have the following forms:

$$F_{s,n} = 1/\sqrt{a} \quad \text{if} \quad n = 0\,, \qquad F_{s,n} = \sqrt{2/a} \quad \text{if} \quad n > 0\,.$$

If q_l and q_t both are real, or if q_l and q_t are pure imaginary ($q_l = ip_l$, $q_t = ip_t$, where p_l and p_t are real numbers), then

$$\begin{aligned} F_d^{-2} = \frac{1}{8q_l q_t} [&2aq_l^3 q_t^5 + 4aq_l^3 q_t^3 q_x^2 + 2aq_l q_t^5 q_x^2 + 10aq_l^3 q_t q_x^4 - 4aq_l q_t^3 q_x^4 + 2aq_l q_t q_x^6 \\ &- 8aq_l^3 q_t q_x^2 (q_t^2 + q_x^2) \cos(aq_l) - 2aq_l q_t (q_t^2 - q_x^2)^2 (q_l^2 + q_x^2) \cos(aq_t) \\ &+ 2q_t(-q_t^2 + q_x^2)(q_l^2 q_t^2 + 7q_l^2 q_x^2 - q_t^2 q_x^2 + q_x^4) \sin(aq_l) \\ &+ 8q_l^3 q_x^2 (q_t^2 - q_x^2) \sin(aq_t) + (q_l^2 q_t^5 + 4q_l^3 q_t^2 q_x^2 + 6q_l^2 q_t^3 q_x^2 \\ &- q_t^5 q_x^2 - 4q_l^3 q_x^4 - 7q_l^2 q_t q_x^4 + 2q_t^3 q_x^4 - q_t q_x^6) \sin(a(q_l - q_t)) \\ &+ (q_l^2 q_t^5 - 4q_l^3 q_t^2 q_x^2 + 6q_l^2 q_t^3 q_x^2 - q_t^5 q_x^2 + 4q_l^3 q_x^4 - 7q_l^2 q_t q_x^4 \\ &+ 2q_t^3 q_x^4 - q_t q_x^6) \sin(a(q_l + q_t))]\,, \end{aligned}$$

$$F_f^{-2} = \frac{1}{8q_l q_t}[2aq_l^3q_t^5 + 4aq_l^3q_t^3q_x^2 + 2aq_lq_t^5q_x^2 + 10aq_l^3q_tq_x^4 - 4aq_lq_t^3q_x^4 + 2aq_lq_tq_x^6$$
$$+ 8aq_l^3q_tq_x^2(q_t^2 + q_x^2)\cos(aq_l) + 2aq_lq_t(q_t^2 - q_x^2)^2(q_l^2 + q_x^2)\cos(aq_t)$$
$$+ 2q_t(q_t^2 - q_x^2)(q_l^2q_t^2 + 7q_l^2q_x^2 - q_t^2q_x^2 + q_x^4)\sin(aq_l)$$
$$+ 8q_l^3q_x^2(-q_t^2 + q_x^2)\sin(aq_t) + (q_l^2q_t^5 + 4q_l^3q_t^2q_x^2 + 6q_l^2q_t^3q_x^2$$
$$- q_t^5q_x^2 - 4q_l^3q_x^4 - 7q_l^2q_tq_x^4 + 2q_t^3q_x^4 - q_tq_x^6)\sin(a(q_l - q_t))$$
$$+ (q_l^2q_t^5 - 4q_l^3q_t^2q_x^2 + 6q_l^2q_t^3q_x^2 - q_t^5q_x^2 + 4q_l^3q_x^4 - 7q_l^2q_tq_x^4$$
$$+ 2q_t^3q_x^4 - q_tq_x^6)\sin(a(q_l + q_t))].$$

If q_l is a pure imaginary number ($q_l = ip_l$, where p_l is a real number) and q_t is a real number, then

$$F_d^{-2} = \frac{1}{4p_l q_t}[-ap_l^3q_t^5 - 2ap_l^3q_t^3q_x^2 + ap_lq_t^5q_x^2 - 5ap_l^3q_tq_x^4 - 2ap_lq_t^3q_x^4 + ap_lq_tq_x^6$$
$$+ 4ap_l^3q_tq_x^2(q_t^2 + q_x^2)\cosh(ap_l) + ap_lq_t(p_l^2 - q_x^2)(q_t^2 - q_x^2)^2\cos(aq_t)$$
$$+ (p_l^2q_t^5 + 6p_l^2q_t^3q_x^2 + q_t^5q_x^2 - 7p_l^2q_tq_x^4 - 2q_t^3q_x^4 + q_tq_x^6)\sinh(ap_l)$$
$$+ 4p_l^3q_x^2(q_x^2 - q_t^2)\sin(aq_t) - 4p_l^3q_x^2(q_x^2 - q_t^2)\cosh(ap_l)\sin(aq_t)$$
$$+ (-p_l^2q_t^5 - 6p_l^2q_t^3q_x^2 - q_t^5q_x^2 + 7p_l^2q_tq_x^4 + 2q_t^3q_x^4 - q_tq_x^6)$$
$$\times \sinh(ap_l)\cos(aq_t)],$$

$$F_f^{-2} = \frac{1}{4p_l q_t}[ap_l^3q_t^5 + 2ap_l^3q_t^3q_x^2 - ap_lq_t^5q_x^2 + 5ap_l^3q_tq_x^4 + 2ap_lq_t^3q_x^4 - ap_lq_tq_x^6$$
$$+ 4ap_l^3q_tq_x^2(q_t^2 + q_x^2)\cosh(ap_l) + ap_lq_t(p_l^2 - q_x^2)(q_t^2 - q_x^2)^2\cos(aq_t)$$
$$+ (p_l^2q_t^5 + 6p_l^2q_t^3q_x^2 + q_t^5q_x^2 - 7p_l^2q_tq_x^4 - 2q_t^3q_x^4 + q_tq_x^6)\sinh(ap_l)$$
$$+ 4p_l^3q_x^2(q_x^2 - q_t^2)\sin(aq_t) + 4p_l^3q_x^2(q_x^2 - q_t^2)\cosh(ap_l)\sin(aq_t)$$
$$+ (p_l^2q_t^5 + 6p_l^2q_t^3q_x^2 + q_t^5q_x^2 - 7p_l^2q_tq_x^4 - 2q_t^3q_x^4 + q_tq_x^6)$$
$$\times \sinh(ap_l)\cos(aq_t)].$$

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