ACOUSTIC PHONON SPECTRUM AND DENSITY OF STATES IN FREE STANDING QUANTUM WELLS

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Abstract

The confined acoustic phonons in free-standing quantum wells are considered. Their spectrum may determined from the dispersion equations. We have developed a special stable algorithm to obtain numerical solutions of these equations. We have calculated the acoustic phonon density of states in a free-standing quantum well. The density of states is , on the average, a quadratic function of energy, however it has singularities corresponding to the extrema in the dispersion relations.

I. INTRODUCTION

In low dimensional microstructures acoustic phonon states may undergo significant modifications due to the quantization in one, two, or three directions. Acoustic phonon confinement will strongly affect the electron and photon interactions with acoustic phonons resulting in peculiarities of electron transport properties and light scattering. Therefore it is necessary to develop an adequate model of acoustic phonon states in low dimensional structures and their interactions with electrons and photons.

In this paper we consider confined acoustic modes in a thin solid slab of isotropic material. We have calculated the confined phonon spectrum and the corresponding density of states (DOS). The equation governing the elastic vibrations in our system is the Navier equation for a relative displacement vector and it is supplemented by appropriate boundary conditions which are the conditions of free (unstressed) surfaces [1, 2, 3]. We have transformed the problem at hand to an eigenvalue equation with a Hermitian matrix differential operator. The solutions of this eigenvalue problem are three different types of modes with different symmetries: shear waves, dilatational waves and flexural waves. Although the general form of the solution may be obtained analytically, it includes several parameters (phonon quantum numbers) which should be determined by numerically solving the system of nonlinear dispersion equations. These phonon quantum numbers are complex valued functions of the in-plane phonon wave vector and they may approach each other so closely for some values of the in-plane wave vector, that the numerical solution of the dispersion equations leaps from one branch to another. We have developed a special stable algorithm to obtain these solutions.

II. CONFINED ACOUSTIC PHONON SPECTRUM

Shear waves have the simplest quantization rules. A vector of relative displacement in shear waves has only one nonzero component in the direction perpendicular to both the direction of propagation and the direction perpendicular to the slab . The dispersion relation for shear waves is

$$\omega_n = s_t \sqrt{q_n^2 + q_{||}^2}\,, \tag{1}$$

where s_t is the transverse sound velocity in the bulk material, $q_{||}$ is an in-plane wave vector, $q_n = (\pi n/a)$, $n = 0, 1, 2, ...$

Dilatational waves and flexural waves have two nonzero components of the vector of relative displacement – in the direction of wave propagation and in the perpendicular to the slab direction. The pattern of the vector of relative displacement is symmetric in respect to the slab midplane for dilatational waves and antisymmetric for flexural waves. The dispersion relations for dilatational waves are given implicitly by the system of equations

$$\omega_n^2 = s_l^2\,(q_{||}^2 + l_n^2) = s_t^2\,(q_{||}^2 + t_n^2)\,, \tag{2}$$

$$\frac{\tan(t_n a/2)}{\tan(l_n a/2)} = -\frac{4q_{||}^2 l_n t_n}{(q_{||}^2 - t_n^2)^2}\,, \tag{3}$$

where s_l is the longitudinal sound velocity in the bulk material, parameters l_n and t_n are determined from equations (2) and (3), which have many solutions as denoted by the index n. The dispersion relations for flexural waves are given implicitly by eq. (2) and the equation

$$\frac{\tan(l_n a/2)}{\tan(t_n a/2)} = -\frac{4q_{||}^2 l_n t_n}{(q_{||}^2 - t_n^2)^2}\,. \tag{4}$$

The graphs of functions $\omega_n(q_{||})$ obtained by numerical solutions of the system of eqs. (1)-(4) is shown in the Fig. 1a, 2a and 3a for shear waves, dilatational waves and flexural waves, respectively. We used elastic constants of $GaAs$ and took the slab width as $a = 100\text{Å}$. These graps are plotted for the 12 lowest modes.

III. ACOUSTIC PHONON DENSITY OF STATES

The peculiarities of the acoustic phonon spectrum will be markedly pronounced in the their density of states (DOS). The DOS of confined phonons is defined by the formula

$$\mathcal{N} = \frac{\mathcal{A}}{(2\pi)^2}\sum_n \int_{\omega_n = const} \frac{dq_{||}}{\left|d\omega_n/dq_{||}\right|}\,, \tag{5}$$

where $\mathcal{A}$ is the area of the slab, and the sum is taken over phonon modes; integral in (5) is taken over the curve of constant energy and $\mathcal{N}$ is a function of the energy.

We have to specify the Brillouin zone to calculate the DOS over a wide range of energy. For a model estimation we accepted a simple square Brillouin zone. So we take into account only those acoustic phonons in integral (5) which have wavevectors inside the first Brillouin zone. The lattice constant is taken equal 5.65Å which corresponds to the case of $GaAs$. The graph of the DOS obtained by numerical calculation of the integral of (5) for shear, dilatational and flexural phonons is depicted in Fig. 1b, 2b, and 3b, respectivelyly. At energies lower than some critical energy (corresponding to the edge of the Brillouin zone) the DOS is, on the average, a quadratic function of energy. This functional dependence occurs when many phonon branches contribute to the DOS and it corresponds to the case of bulk acoustic phonons. It is obscured in Fig. 1b, 2b, and 3b because the graphs are plotted in the semilogarithmic scale to emphasize the singularities of the DOS. These singularities correspond to the extrema in the dispersion relation; formally the DOS goes to infinity in such points. In Fig. 1b, 2b, and 3b, the DOS is plotted for energies up to $10\,meV$. At higher energies the finiteness of the Brillouin zone becomes important and the function $\mathcal{N}$ saturates in the average.

The DOS may be determined experimentally from neutron scattering spectra [4, 5] or from Brillouin light scattering spectra [6, 7]. It is a very important function characterizing the acoustic phonon subsystem and determining peculiarities of phonon interactions with phonons, photons and electrons. The singular points of the DOS make the observing conditions for the neutron scattering spectra and the Brillouin light scattering spectra more favorable, because the intensity of the scattered (reflected) radiation is proportional to the DOS of acoustic phonons.

IV. CONCLUSIONS

We have calculated the acoustic phonon modes and their density of states in free-standing quantum wells. The density of states has singularities related to the extrema of the acoustic phonon dispersion law. In these singular points the DOS formally goes to infinity. It makes the observing conditions for light and neutron scattering spectra more favorable.

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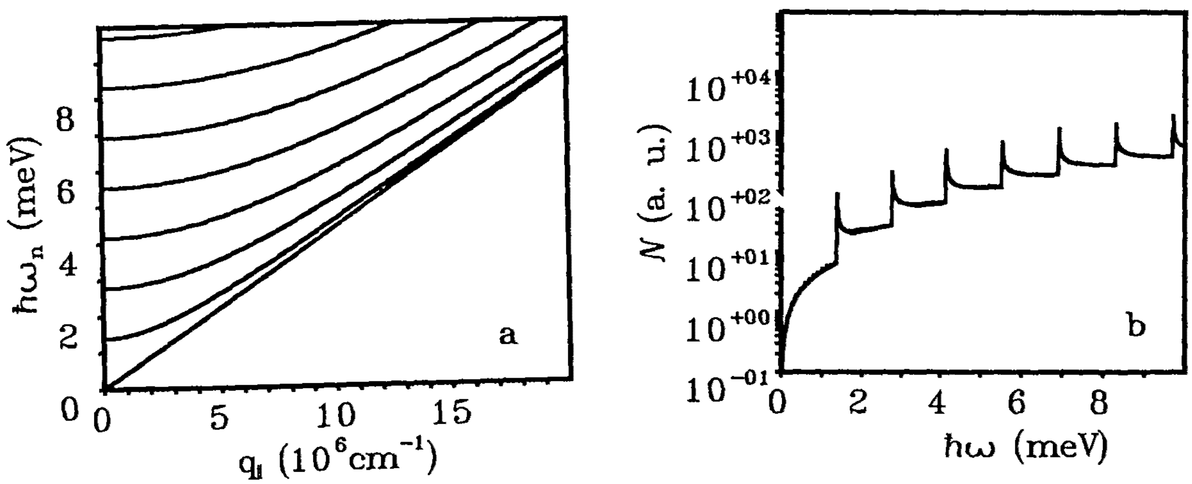

Figure 1. The dependences of the phonon energy, $\hbar\omega_n$, on the in-plane wavevector, $q_{\|}$, (a) and the density of states, $\mathcal{N}$, on the phonon energy, $\hbar\omega$, (b) for shear phonons in a free-standing *GaAs* quantum well of width 100Å.

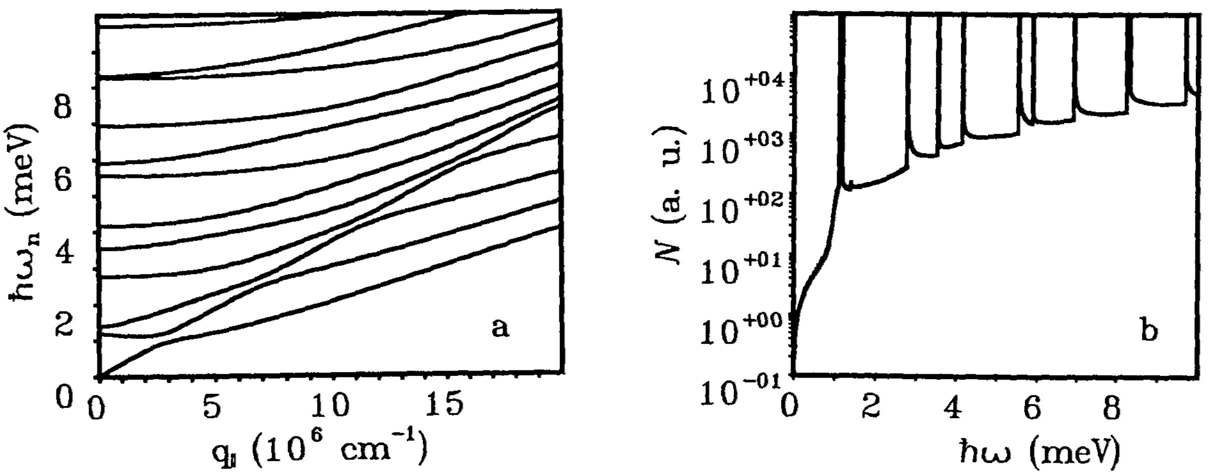

Figure 2. The dependences of the phonon energy, $\hbar\omega_n$, on the in-plane wavevector, $q_{\parallel}$, (a) and the density of states, $\mathcal{N}$, on the phonon energy, $\hbar\omega$, (b) for dilatational phonons in a free-standing *GaAs* quantum well of width 100Å.

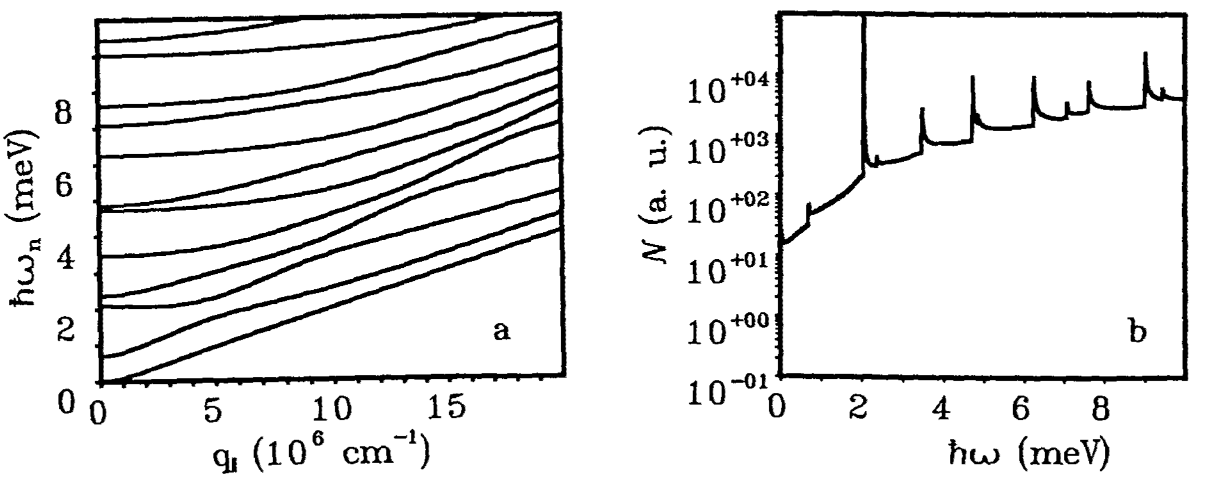

Figure 3. The dependences of the phonon energy, $\hbar\omega_n$, on the in-plane wavevector, $q_{\parallel}$, (a) and the density of states, $\mathcal{N}$, on the phonon energy, $\hbar\omega$, (b) for flexural phonons in a free-standing *GaAs* quantum well of width 100Å.