Novi Sad J. Math.
Vol. 30, No. 3, 2000, 185-190

PHONON SPECTRA OF QUANTUM WIRES

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Abstract

This paper based on our previous works which dealth with ultrathin crystalline films. The quantum wires are quasi $1D$ crystalline systems bounded in two perpendicular directions (y and z) while infinite in the x direction. The phonon excitation energies are defined by the poles of Green's functions, which be found from the condition that the $3D$ determinant of the set of equation of motion vanishes. Using Chebyshev's polynomial representation of this block matrix, we obtain the solutions as roots of the characteristic matrix equation. By numerical analysis (for simplest cases: $N_{y/z} \in [2,5]$) we conjectured that the solution of this equation is of the same form as for thin films, but with the discretization along the y direction too.

AMS MAthematics Subject Classification (1991): 65F40, 81T25
Key words and phrases: phonons, quantum wires, Green's functions, dispersion relations

We tried to study the basic microscopic behaviour of the phonon subsystem in quantum wires which are of particular importance regarding its influence on macroscopic properties that are connected with their possible application in nanotechnology [1]-[7]. This paper is based on our previous works which dealt ultrathin films [8]-[12]. Contrary to thin films which are quasi $2D$ systems bounded by two surfaces parallel to the XY planes, quantum wires are quasi $1D$ crystalline systems bounded in two directions (y and z).

The phonon dispersion law can be derived using Green's function method [13]-[17]. We use the following two-time temperature dependent retarded Green's function:

$$G^{\alpha\alpha}_{\vec{n},\vec{m}}(t) \equiv \langle\langle u^{\alpha}_{\vec{n}}(t)|u^{\alpha}_{\vec{m}}(0)\rangle\rangle = \Theta(t)\langle[u^{\alpha}_{\vec{n}}(t), u^{\alpha}_{\vec{m}}(0)]\rangle_0 \tag{1}$$

where $u^{\alpha}_{\vec{n}}$ is the displacement of an atom at the site $\vec{n} \equiv (n_x n_y n_z)$ in the α direction ($\alpha \in \{x, y, z\}$). Finding the second derivative, we get the equation of motion for Green's function:

$$M_{\vec{n}}\frac{d^2}{dt^2}G^{\alpha\alpha}_{\vec{n},\vec{m}}(t) = -i\hbar\delta_{\vec{n}\vec{m}}\delta(t) + \frac{\Theta(t)}{i\hbar}\langle[[p^{\alpha}_{\vec{n}}, H(t)]\,, u^{\alpha}_{\vec{m}}(0)]\rangle_0\,. \tag{2}$$

The Hamiltonian of the phonon subsystem in the harmonic and nearest neighbour approximation (neglecting torsion constants $C^{\alpha\neq\beta}$, see in [8] - [10]) is:

$$\begin{aligned} H = \frac{1}{4}\sum_{n_x n_y n_z;\alpha} \Big[& 2M_{n_x n_y n_z}\dot{u}^2_{n_x n_y n_z;\alpha} + C^{\alpha\alpha}_{n_x n_y n_z;n_x\pm1,n_y n_z}\cdot \\ & \cdot\left(u^{\alpha}_{n_x n_y n_z} - u^{\alpha}_{n_x\pm1,n_y n_z}\right)^2 C^{\alpha\alpha}_{n_x n_y n_z;n_x n_y\pm1,n_z}\left(u^{\alpha}_{n_x n_y n_z} - u^{\alpha}_{n_x n_y\pm1,n_z}\right)^2 + \\ & + C^{\alpha\alpha}_{n_x n_y n_z;n_x n_y n_z\pm1}\left(u^{\alpha}_{n_x n_y n_z} - u^{\alpha}_{n_x n_y n_z\pm1}\right)^2\Big]\,. \end{aligned} \tag{3}$$

Performing time Fourier transform and simplifying the model, assuming $M_{\vec{n}} \equiv M$ and $C^{\alpha\alpha}_{\vec{n},\vec{n}+\vec{\lambda}_{x/y/z}} \equiv C^{\alpha\alpha}_{x/y/z}$, and calculating the commutators $[p^{\alpha}_{n_x n_y n_z}, H]$, the equation of motion for Green's function turns into:

$$\begin{aligned} M\omega^2 G^{\alpha\alpha}_{n_x n_y n_z;m_x m_y m_z}(\omega) = \frac{i\hbar}{2\pi}\delta_{n_x n_y n_z;m_x m_y m_z} + \\ + \Big[C^{\alpha\alpha}_x\left(G^{\alpha\alpha}_{n_x n_y n_z;m_x m_y m_z} - G^{\alpha\alpha}_{n_x\pm1,n_y n_z;m_x m_y m_z}\right) + C^{\alpha\alpha}_y\left(G^{\alpha\alpha}_{n_x n_y n_z;m_x m_y m_z} - \right. \\ \left. - G^{\alpha\alpha}_{n_x n_y\pm1,n_z;m_x m_y m_z}\right) + C^{\alpha\alpha}_z\left(G^{\alpha\alpha}_{n_x n_y n_z;m_x m_y m_z} - G^{\alpha\alpha}_{n_x n_y n_z\pm1;m_x m_y m_z}\right)\Big] \end{aligned} \tag{4}$$

(see [12], [16]). One can use this equation to analyze the phonon subsystem both in ideal infinite crystals and in bounded crystalline systems (films and quantum wires), because of its general character.

The equation for Green's function must be amended with the conditions which describe spatial constraints of the quantum wires:

$$u^{\alpha}_{n_x n_y n_z} = 0 \,, \quad G^{\alpha\alpha}_{n_x n_y n_z; m_x m_y m_z}(\omega) = 0 \,; \quad \text{for} \left\{ \begin{array}{l} n_y < 0 \text{ and } n_y > N_y \\ n_z < 0 \text{ and } n_z > N_z \end{array} \right\} \tag{5}$$

One gets the systems of $(N_y + 1) \times (N_z + 1)$ equations. Performing partial spatial Fourier transform (because of the breaking of translational invariance along the (y, z) directions, see [12], [16], [17]), we obtain the systems of $(N_y+1) \times (N_z+1)$ inhomogenious algebraic difference equations:

$$\begin{aligned} & b\left(G^{\alpha\alpha}_{n_y-1,n_z;m_y m_z} + G^{\alpha\alpha}_{n_y+1,n_z;m_y m_z}\right) + c\left(G^{\alpha\alpha}_{n_y n_z-1;m_y m_z} + G^{\alpha\alpha}_{n_y n_z+1;m_y m_z}\right) + \\ & \qquad + \rho G^{\alpha\alpha}_{n_y n_z;m_y m_z} = \mathcal{K}_{n_y n_z;m_y m_z} \,, \end{aligned} \tag{6}$$

where:

$$\rho = -2 + \frac{1}{\left(\Omega^{\alpha\alpha}_y\right)^2 + (\Omega^{\alpha\alpha}_z)^2}\left[\omega^2 - 4\,(\Omega^{\alpha\alpha}_x)^2 \sin^2 \frac{a_x k_x}{2}\right] \,; \tag{7}$$

$$b = \frac{\left(\Omega^{\alpha\alpha}_y\right)^2}{\left(\Omega^{\alpha\alpha}_y\right)^2 + (\Omega^{\alpha\alpha}_z)^2} \,; \quad c = \frac{(\Omega^{\alpha\alpha}_z)^2}{\left(\Omega^{\alpha\alpha}_y\right)^2 + (\Omega^{\alpha\alpha}_z)^2} \,;$$

$$\mathcal{K}_{n_y n_z;m_y m_z} \equiv \frac{i\hbar\, \delta_{n_y n_z;m_y m_z}}{2\pi \cdot \left[\left(\Omega^{\alpha\alpha}_y\right)^2 + (\Omega^{\alpha\alpha}_z)^2\right]} \,.$$

In the case of quantum wires we replace two and three index counting by single index counting using the following substitutions: $l = n_z + 1 + (N_z + 1)\, n_y$. The systems of equations for determining Green's function are transformed into more practical form:

$$b\left[G^{\alpha\alpha}_{l-(N_z+1)} + G^{\alpha\alpha}_{l+(N_z+1)}\right] + c\left(G^{\alpha\alpha}_{l-1} + G^{\alpha\alpha}_{l+1}\right) + \rho G^{\alpha\alpha}_l = \mathcal{K}_l \,; \tag{8}$$

$$l \in [1, (N_y + 1) \times (N_z + 1)] \,.$$

We can express Green's function as $G^{\alpha\alpha}_l = \dfrac{D_l}{D}$, where D is the determinant of these systems of equations. As the poles of Green's function determine phonon excitation energies [12] - [17] the problem reduces to the finding of the roots of the characteristic polynomials of these determinants:

$$D=\begin{vmatrix} R & B & O & \cdots & O & O & O \\ B & R & B & \cdots & O & O & O \\ O & B & R & \cdots & O & O & O \\ \\ . & . & . & \ddots & . & . & . \\ \\ O & O & O & \cdots & R & B & O \\ O & O & O & \cdots & B & R & B \\ O & O & O & \cdots & O & B & R \end{vmatrix}_{N_y+1} \qquad R=\begin{bmatrix} \rho & c & 0 & \cdots & 0 & 0 & 0 \\ c & \rho & c & \cdots & 0 & 0 & 0 \\ 0 & c & \rho & \cdots & 0 & 0 & 0 \\ \\ . & . & . & \ddots & . & . & . \\ \\ 0 & 0 & 0 & \cdots & \rho & c & 0 \\ 0 & 0 & 0 & \cdots & c & \rho & c \\ 0 & 0 & 0 & \cdots & 0 & c & \rho \end{bmatrix}_{N_z+1}$$

(9)

where $B = \operatorname{diag}[b]_{N_z+1}$ and O is a $2D$ zero-matrix.

The analytic results for phonon spectra in films:

$$\omega^{\alpha\alpha}_{k_xk_yn_z/f} = 2\left[\Omega^{\alpha\alpha}_x \sin^2 \tfrac{a_xk_x}{2} + \Omega^{\alpha\alpha}_y \sin^2 \tfrac{a_yk_y}{2} + \Omega^{\alpha\alpha}_z \sin^2 \tfrac{\pi\nu_z}{2(N_z+2)}\right]^{1/2}$$

(10)

has already been presented in our previous works [12], [18]. By numerical analysis of the quantum wires problem we conjectured analytic forms of the dispersion laws in these crystal structures:

$$\omega^{\alpha\alpha}_{k_xk_yn_z/w} = 2\left[\Omega^{\alpha\alpha}_x \sin^2 \frac{a_xk_x}{2} + \Omega^{\alpha\alpha}_y \sin^2 \frac{\pi\nu_y}{2(N_y+2)} + \Omega^{\alpha\alpha}_z \sin^2 \frac{\pi\nu_z}{2(N_z+2)}\right]^{1/2}.$$

(11)

The quantum numbers ν_α, $\alpha = (y,z)$ from expressions (10) and (11) take the values: $\nu_\alpha \in [1, N_\alpha + 1]$. One can see that the solutions have the form of Pitagora's theorem and that the discretization of the spectrum along one direction is independent of the discretization the along other directions.

The dispersion laws (10) in thin films and (11) in quantum wires are formally of the same form as in the corresponding infinite ideal crystal. The main difference is the appearance of discretization of phonon energies along directons that are spatially bounded.

The most important result of these analises is the existence of energy gaps in bounded structures. Because its appearance is a consequence of the breaking of translational symmetry (along bounded directions), the gap values are greater in quantum wires than in thin films, while in unbounded crystals its values are neglected.

From (10) and (11) one can write the expresssion for the energy gaps in low-dimensional crystal systems as:

$$g_{f/w}^{\alpha\alpha} \approx \pi \left[\sum_{\beta \in \{x,y,z\}} \left(\Omega_{\beta}^{\alpha\alpha} \frac{\nu_{min}^{\beta}}{N_\beta + 2} \right)^2 \right]^{1/2} \tag{12}$$

where: $\nu_{min}^x = \nu_{min}^y = 0$, $\nu_{min}^z = 1$ for films and $\nu_{min}^x = 0$, $\nu_{min}^y = \nu_{min}^z = 1$ for wires.

One can see from (12) that the values of the gaps show a sharp decrease sharply (almost hyperbolical) with the increase of the size of the system, i.e. with the increase of N_β.

The presence of the gaps in the phonon spectra cannot be explained by the disappearance of acoustic and appearance of the optical phonons ([8]-[10], [19], [20]), for in our model we analyzed only the simple cubic lattice. The possible explanation is the appearance of acoustic phonons of optical type [12], [18]. This explanation can be supported by the calculation of the statistical limit, i.e. $\lim_{N_{y/z} \to \infty} g_{f/w}^{\alpha\alpha} = 0$.

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