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Confined bulklike longitudinal optical phonon modes in right triangular quantum dots and quantum wires

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Abstract
Under the dielectric continuum model, the confined bulklike longitudinal optical phonon modes and electron–optical-phonon interaction of the isosceles right triangular (45°–45°–90°) quantum dot (wire) and hemi-equilateral triangular (30°–60°–90°) quantum dot (wire) are studied. The analytical expressions for the confined bulklike longitudinal optical phonon eigenfunctions are deduced. After having quantized the polarization eigenvectors, we derive the Hamiltonian operators describing the confined bulklike longitudinal optical phonon modes and their interactions with electrons. The potential applications of these results are also discussed.

1. Introduction

In recent years, many methods such as metal-organic chemical vapour deposition, molecular beam epitaxy, and vapour–liquid–solid growth have been developed for fabricating nanomaterials with a wide range of sizes, shapes, and dielectric environments. PbSe, CdS, and NiS triangular nanoprisms (nanotriangles) [1–3], and GaN and n-GaN/InGaN/p-GaN triangular nanowires [4, 5] have been synthesized. Because of the special physical properties, they show successful and potential applications in a wide variety of fields, such as nanowire lasers [6], optical biosensors [7] and photothermal agents [8]. The optoelectronic and physicochemical properties of nanomaterials are a strong function of particle size. The nanomaterials shape also contributes significantly to modulating their physical properties. Nanomaterials of different shapes have different crystallographic facets and different fractions of surface atoms on their corners and edges, which makes it interesting to research the effect of shape on their physical properties. On the other hand, the polar vibration modes and electron–phonon interaction play a key role in many physical properties of polar crystals, such as the binding energy of impurities, carrier transportation, linear and non-linear optical properties, especially in low-dimensional materials. Hence, an analytic description of polar optical phonon modes and the electron–phonon interaction Hamiltonian for quantum systems of complex shapes is essential.

There are several theoretical models, such as the dielectric continuum model [9–13], hydrodynamic model [14], and microscopic calculation model [15, 16] used for studying phonon modes and electron–phonon interaction in various low-dimensional quantum systems. The dielectric continuum model has been widely used for its simplicity and efficiency. Mori and Ando [17] deduced the phonon modes in single and double heterostructures. Knipp and Reinecke [18] studied the interface optical (IO) phonon modes in a quantum wire with elliptical cross sections. Xie *et al* [19, 20] determined the IO and surface optical (SO) phonon modes in a free-standing cylindrical quantum wire and an embedded quantum well wire. Klein *et al* [21] and Roca *et al* [22] derived the polar optical phonon modes in a spherical quantum dot. de la Cruz *et al* [23] obtained the IO phonon mode in a GaAs/$Al_xGa_{1-x}As$ spherical quantum dot. Shi *et al* [24, 25] studied both the IO and propagating optical phonon modes in wurtzite GaN/$Al_xGa_{1-x}N$ quantum wells. Li and Chen [26] deduced the confined bulklike longitudinal optical (LO), top surface optical (TSO) and side surface optical (SSO) phonon modes in a cylindrical quantum dot. Zhang *et al* [27] derived the phonon modes in a quantum dot quantum well. Kanyinda-Malu *et al* [28] derived the axial interface optical phonon modes in a double-nanoshell system. Wu and Xie [29] worked out the confined bulklike LO, TSO and SSO phonon

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modes in a quantum annulus. Recently, we [30] studied the confined bulklike LO phonon modes in the equilateral triangular quantum dot and quantum wire. In this paper, we extend the previous work to the isosceles right triangular (45°–45°–90°) quantum dot (wire) and hemi-equilateral triangular (30°–60°–90°) quantum dot (wire) systems.

The paper is organized as follows: in section 2, the confined bulklike LO phonon modes and the corresponding Fröhlich electron–phonon interaction Hamiltonian of the isosceles right triangular quantum dot (IRTQD) and quantum wire (IRTQW) are deduced. In section 3, by the theoretical scheme of the IRTQD and IRTQW, we derive the confined bulklike LO phonon modes and the corresponding Fröhlich electron–phonon interaction Hamiltonian of the hemi-equilateral triangular quantum dot (HETQD) and quantum wire (HETQW). In section 4, the potential applications of these results are discussed.

2. The confined bulklike LO phonon modes of the IRTQD and the IRTQW

Under the dielectric continuum approximation, we start with the electrostatic equations

$$\mathbf{E} = -\nabla\phi(\mathbf{r}), \tag{1}$$

$$\mathbf{D} = \varepsilon\mathbf{E} = \mathbf{E} + 4\pi\mathbf{P}, \tag{2}$$

$$\nabla\cdot\mathbf{D} = 4\pi\rho_0(\mathbf{r}), \tag{3}$$

where $\mathbf{D}$, $\mathbf{E}$ and $\mathbf{P}$ are the electric displacement, electric field strength and electric polarization density, respectively. ϕ, ρ_0 and ε are the electric potential, the free charge density and the dielectric constant, respectively. For free oscillation, the charge density $\rho_0(\mathbf{r}) = 0$, so we get the following equation

$$\varepsilon\nabla^2\phi(\mathbf{r}) = 0. \tag{4}$$

There are two possible solutions for equation (4), one of which is

$$\varepsilon(\omega) = 0, \tag{5}$$

the other is

$$\nabla^2\phi(\mathbf{r}) = 0. \tag{6}$$

In this paper, we only focus on the first solution. Since in a polar crystal,

$$\varepsilon(\omega) = \varepsilon_\infty + \frac{\varepsilon_0 - \varepsilon_\infty}{1 - \omega^2/\omega_{\mathrm{TO}}^2}, \tag{7}$$

where ε_0, ε_∞ are the static and high-frequency dielectric constants and ω_{TO} is the frequency of the transverse optical phonon, $\varepsilon(\omega) = 0$ would give

$$\omega^2 = \omega_{\mathrm{TO}}^2\frac{\varepsilon_0}{\varepsilon_\infty} = \omega_{\mathrm{LO}}^2. \tag{8}$$

Equation (8) is just the Lyddane–Sachs–Teller (LST) relation, which describes the confined bulklike LO phonon vibration modes of frequency $\omega = \omega_{\mathrm{LO}}$.

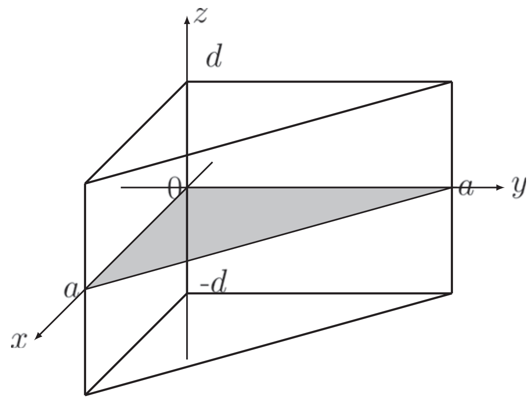

Figure 1. The geometry of the IRTQD.

2.1. The confined bulklike LO phonon modes of the IRTQD

Firstly, we investigate an IRTQD of a polar semiconductor placed in a vacuum. The geometry of the IRTQD is shown in figure 1. The height is $2d$. The IRTQD cross section has side lengths a. The dielectric constant is assumed to be isotropic.

In the IRTQD, the electric potential $\phi(\mathbf{r})$ in equation (4) is an arbitrary function of x, y, z. Owing to the electrostatic boundary conditions that the tangential component of $\mathbf{E}$ and the normal component of $\mathbf{D}$ are continuous at the boundary and equation (5), the electric potential $\phi(\mathbf{r})$ should be zero at the boundary and in the region outside. According to the geometry of the quantum dot, the electric potential $\phi(\mathbf{r})$ can be taken as

$$\phi(\mathbf{r}) = \Psi(x, y)f(z), \tag{9}$$

$$f(z) = \begin{cases} C\cos(k_z z) + D\sin(k_z z) & \text{for } -d \leqslant z \leqslant d, \\ 0 & \text{otherwise,} \end{cases} \tag{10}$$

where k_z is the phonon wavevector in the z direction. C, D and k_z are to be determined by the boundary conditions. Since the plane $z = 0$ possesses reflectional symmetry, the electrostatic potential should be either symmetric or antisymmetric about this plane. The boundary conditions match in two ways: either $C = 0$ or $D = 0$. So, we have two solutions for $f(z)$:

$$f^S(z) = C\cos\left(\frac{n\pi}{2d}z\right), \qquad n = 1, 3, 5, \ldots, \tag{11}$$

and

$$f^A(z) = D\sin\left(\frac{n\pi}{2d}z\right), \qquad n = 2, 4, 6, \ldots. \tag{12}$$

However, the IRTQD cross section function $\Psi(x, y)$ is not solvable by a separation of variables. As a matter of fact, the cross section function problem is similar to the quantum mechanical problem of a particle in an isosceles right triangle (billiard). On the other hand, the isosceles right triangle can be obtained by subdividing a square along a diagonal. The eigenfunctions of an isosceles right triangle can be deduced by linear combinations of these solutions of the square, which can be found in these articles [31–33]. In this paper, we use the results of Li [31].

$$\Psi^{+}_{lm}(x,y) = \frac{1}{\sqrt{2}}\left[\sin\left(\frac{l\pi x}{a}\right)\sin\left(\frac{m\pi y}{a}\right) + \sin\left(\frac{m\pi x}{a}\right)\sin\left(\frac{l\pi y}{a}\right)\right], \quad (13)$$

where $m = 1, 2, 3, \ldots, l = m+1, m+3, \ldots$, and

$$\Psi^{-}_{lm}(x,y) = \frac{1}{\sqrt{2}}\left[\sin\left(\frac{l\pi x}{a}\right)\sin\left(\frac{m\pi y}{a}\right) - \sin\left(\frac{m\pi x}{a}\right)\sin\left(\frac{l\pi y}{a}\right)\right], \quad (14)$$

where $m = 1, 2, 3, \ldots, l = m+2, m+4, \ldots$.

So, the eigenfunctions of the confined bulklike LO phonons can be chosen as

$$\phi^{S+}_{lmn} = \begin{cases} C_{lmn}\Psi^{+}_{lm}(x,y) f^{S}(z) & \text{in IRTQD,} \\ 0 & \text{otherwise,} \end{cases} \quad (15)$$

$$\phi^{S-}_{lmn} = \begin{cases} C_{lmn}\Psi^{-}_{lm}(x,y) f^{S}(z) & \text{in IRTQD,} \\ 0 & \text{otherwise,} \end{cases} \quad (16)$$

for $n = 1, 3, 5, \ldots$, and

$$\phi^{A+}_{lmn} = \begin{cases} C_{lmn}\Psi^{+}_{lm}(x,y) f^{A}(z) & \text{in IRTQD,} \\ 0 & \text{otherwise,} \end{cases} \quad (17)$$

$$\phi^{A-}_{lmn} = \begin{cases} C_{lmn}\Psi^{-}_{lm}(x,y) f^{A}(z) & \text{in IRTQD,} \\ 0 & \text{otherwise,} \end{cases} \quad (18)$$

for $n = 2, 4, 6, \ldots$.

The polarization vectors for the confined bulklike LO mode are calculated by considering equations (1) and (2) with the condition $\varepsilon = 0$. We get

$$\mathbf{P}^{\sigma}_{lmn} = \frac{1}{4\pi}\nabla\phi^{\sigma}_{lmn}, \qquad \sigma = S+, S-, A+, A-. \quad (19)$$

To derive the expression for the Hamiltonian of the free-phonon field, we start with the dynamic equations of motion of the crystal lattice [11]

$$\mu\ddot{\mathbf{u}} = -\mu\omega_0^2\mathbf{u} + e\mathbf{E}_{\mathrm{loc}}, \quad (20)$$

$$\mathbf{P} = n_p e\mathbf{u} + n_p\alpha\mathbf{E}_{\mathrm{loc}}, \quad (21)$$

where $\mu = m_+m_-/(m_+ + m_-)$, $\mathbf{u} = \mathbf{u}_+ - \mathbf{u}_-$, ω_0 and n_p are the reduced mass of the ion pair, the relative displacement of the positive and negative ions, the frequency associated with the short-range force between ions and the number of ion pairs per unit volume, respectively. α, $\mathbf{E}_{\mathrm{loc}}$ and $\mathbf{P}$ are the electronic polarizability per ion pair, the local field at the position of the ions and the polarization field produced by the oscillating ions, respectively. The Hamiltonian of the free vibration is given by

$$H_{\mathrm{ph}} = \tfrac{1}{2}\int\left[n_p\mu\dot{\mathbf{u}}\cdot\dot{\mathbf{u}} + n_p\mu\omega_0^2\mathbf{u}\cdot\mathbf{u} - n_p e\mathbf{u}\cdot\mathbf{E}_{\mathrm{loc}}\right]\mathrm{d}^3r. \quad (22)$$

Using the well-known Lorentz relation $\mathbf{E}_{\mathrm{loc}} = \mathbf{E} + 4\pi\mathbf{P}/3$ and the relation $\mathbf{E} = -4\pi\mathbf{P}$, we have

$$\mathbf{E}_{\mathrm{loc}} = -\tfrac{8}{3}\pi\mathbf{P}, \quad (23)$$

$$\mathbf{u} = \frac{1 + \frac{8}{3}\pi n_p\alpha}{n_p e}\mathbf{P}. \quad (24)$$

Substituting equations (23) and (24) into equation (20), we can obtain

$$\ddot{\mathbf{u}} + \omega_{\mathrm{LO}}^2\mathbf{u} = 0, \quad (25)$$

where

$$\omega_{\mathrm{LO}}^2 = \omega_0^2 + \frac{8}{3}\frac{\pi n_p e^2/\mu}{1 + \frac{8}{3}\pi n_p\alpha}. \quad (26)$$

Hence, the confined bulklike LO phonon Hamiltonian from equation (22) can be written as

$$H_{\mathrm{LO}} = \frac{1}{2}\int\left[n_p\mu\left(\frac{1 + \frac{8}{3}\pi n_p\alpha}{n_p e}\right)^2 (\dot{\mathbf{P}}^*\cdot\dot{\mathbf{P}} + \omega_{\mathrm{LO}}^2\mathbf{P}^*\cdot\mathbf{P})\right]\mathrm{d}^3r. \quad (27)$$

The confined bulklike LO polarization vectors form an orthonormal set

$$\int \mathbf{P}^{\sigma'*}_{l'm'n'}\cdot\mathbf{P}^{\sigma}_{lmn}\,\mathrm{d}^3r = \frac{1}{16\pi^2}\int\nabla\phi^{\sigma'*}_{l'm'n'}\cdot\nabla\phi^{\sigma}_{lmn}\,\mathrm{d}^3r = \frac{-1}{16\pi^2}\int\phi^{\sigma'*}_{l'm'n'}\nabla^2\phi^{\sigma}_{lmn}\,\mathrm{d}^3r, \quad (28)$$

in which we use Green's first identity:

$$\int_V \nabla\phi\cdot\nabla\varphi\,\mathrm{d}^3r = -\int_V\phi\nabla^2\varphi\,\mathrm{d}^3r + \int_S\phi\frac{\partial\varphi}{\partial n}\,\mathrm{d}S. \quad (29)$$

In our case $\phi \equiv 0$ (on the boundary), so that the second term equals zero. We get

$$\int \mathbf{P}^{\sigma'*}_{l'm'n'}\cdot\mathbf{P}^{\sigma}_{lmn}\,\mathrm{d}^3r = \frac{[4(l^2+m^2)d^2 + n^2a^2]}{512d}\delta_{\sigma\sigma'}\delta_{ll'}\delta_{mm'}\delta_{nn'}. \quad (30)$$

If we choose C_{lmn} to be

$$C^2_{lmn} = \frac{256d}{n_p\mu[4(l^2+m^2)d^2 + n^2a^2]}\left(\frac{n_p e}{1 + \frac{8}{3}\pi n_p\alpha}\right)^2 = \frac{64d\omega_{\mathrm{LO}}^2}{\pi[4(l^2+m^2)d^2 + n^2a^2]}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right), \quad (31)$$

in which we use the ω_{TO} relation [11]

$$\omega_{\mathrm{TO}}^2 = \omega_0^2 - \frac{4}{3}\frac{\pi n_p e^2/\mu}{1 - \frac{4}{3}\pi n_p\alpha}, \quad (32)$$

and the Clausius–Mossotti relation

$$\varepsilon_\infty = 1 + \frac{4\pi n_p\alpha}{1 - \frac{4}{3}\pi n_p\alpha}, \quad (33)$$

then the confined bulklike LO polarization vectors may form an orthonormal and complete set. We can express the polarization field $\mathbf{P}$ in terms of the complete set of orthonormal polarization modes $\mathbf{P}^{\sigma}_{lmn}$

$$\mathbf{P} = \sum_{lmn}\left(\frac{\hbar}{\omega_{\mathrm{LO}}}\right)^{\frac{1}{2}}(a^{\dagger}_{lmn} + a_{lmn})\mathbf{P}_{lmn}, \quad (34)$$

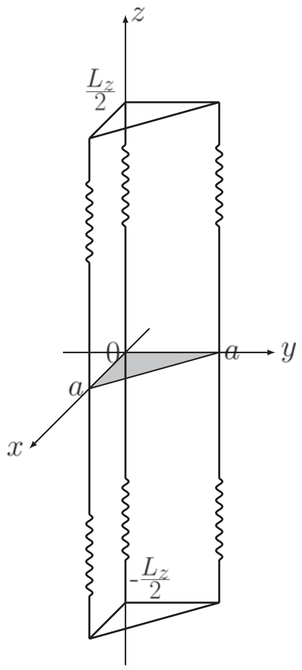

Figure 2. The geometry of the IRTQW.

$$\dot{\mathbf{P}} = -\mathrm{i}\sum_{lmn}(\hbar\omega_{\mathrm{LO}})^{\frac{1}{2}}(a^{\dagger}_{lmn} - a_{lmn})\mathbf{P}_{lmn}, \quad (35)$$

where $\mathbf{P}$ and $\dot{\mathbf{P}}$ are now quantum field operators. $a^{\dagger}_{lmn}$ and a_{lmn} are creation and annihilation operators for the confined bulklike LO phonon of the (l, m, n)th mode. They satisfy the boson commutation relation

$$[a_{lmn}, a^{\dagger}_{l'm'n'}] = \delta_{ll'}\delta_{mm'}\delta_{nn'}, \quad (36)$$

$$[a_{lmn}, a_{l'm'n'}] = [a^{\dagger}_{lmn}, a^{\dagger}_{l'm'n'}] = 0. \quad (37)$$

Hence, from equations (34)–(37), the Hamiltonian operator for the confined bulklike LO phonon becomes

$$H_{\mathrm{LO}} = \sum_{lmn}\hbar\omega_{\mathrm{LO}}(a^{\dagger}_{lmn}a_{lmn} + \tfrac{1}{2}). \quad (38)$$

The electric potential can be expanded as

$$\phi_{\mathrm{LO}} = \sum_{lmn}\left(\frac{\hbar}{\omega_{\mathrm{LO}}}\right)^{\frac{1}{2}}(a_{lmn}\phi^{\sigma}_{lmn} + \mathrm{h.c}), \quad (39)$$

where h.c means the hermitian conjugate.

The Fröhlich Hamiltonian between the electron and the confined bulklike LO phonon can then be written as

$$H_{\mathrm{e-LO}} = -e\phi_{\mathrm{LO}} = -\sum_{lmn}(\Gamma_{lmn}a^{\dagger}_{lmn}\phi^{\sigma}_{lmn} + \mathrm{h.c}), \quad (40)$$

where

$$\Gamma^2_{lmn} = \frac{64de^2\hbar\omega_{\mathrm{LO}}}{\pi[4(l^2+m^2)d^2 + n^2a^2]}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right). \quad (41)$$

2.2. The confined bulklike LO phonon modes of the IRTQW

For the IRTQW, a parallel development is possible for the determination of the confined bulklike LO phonon mode. Since the IRTQW (see the figure 2) has a translational symmetry along the z direction, the eigenfunctions of the confined bulklike LO phonons can be chosen as

$$\phi_{lmk} = \begin{cases} C_{lmk}\Psi^{\pm}_{lm}(x, y)\mathrm{e}^{\mathrm{i}kz} & \text{in IRTQW,} \\ 0 & \text{otherwise,} \end{cases} \quad (42)$$

where k is the phonon wavevector in the z direction. The polarization vectors for the confined bulklike LO mode are

$$\mathbf{P}^{\pm}_{lmk} = \frac{1}{4\pi}\nabla\phi^{\pm}_{lmk}. \quad (43)$$

The confined bulklike LO polarization vectors form an orthonormal and complete set:

$$\int 2n_p\mu\left(\frac{1+\frac{8}{3}\pi n_p\alpha}{n_pe}\right)^2 \mathbf{P}^{i*}_{l'm'k'}\cdot\mathbf{P}^{j}_{lmk}\,\mathrm{d}^3r = \delta_{ij}\delta_{ll'}\delta_{mm'}\delta_{kk'}, \quad (44)$$

$$C^2_{lmk} = \frac{64\pi^2}{L_zn_p\mu[(l^2+m^2)\pi^2 + k^2a^2]}\left(\frac{n_pe}{1+\frac{8}{3}\pi n_p\alpha}\right)^2 = \frac{16\pi\omega^2_{\mathrm{LO}}}{L_z[(l^2+m^2)\pi^2+k^2a^2]}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right), \quad (45)$$

where L_z is the length of the IRTQW.

The polarization field $\mathbf{P}$ can be expressed in terms of the complete set of orthonormal polarization modes $\mathbf{P}^{\pm}_{lmk}$

$$\mathbf{P} = \sum_{lmk}\left(\frac{\hbar}{\omega_{\mathrm{LO}}}\right)^{\frac{1}{2}}(a^{\dagger}_{lmk} + a_{lmk})\mathbf{P}_{lmk}, \quad (46)$$

$$\dot{\mathbf{P}} = -\mathrm{i}\sum_{lmk}(\hbar\omega_{\mathrm{LO}})^{\frac{1}{2}}(a^{\dagger}_{lmk} - a_{lmk})\mathbf{P}_{lmk}, \quad (47)$$

where $\mathbf{P}$ and $\dot{\mathbf{P}}$ are now quantum field operators. $a^{\dagger}_{lmk}$ and a_{lmk} are creation and annihilation operators for the LO phonon of the (l, m, k)th mode. They satisfy the boson commutation relation

$$[a_{lmk}, a^{\dagger}_{l'm'k'}] = \delta_{ll'}\delta_{mm'}\delta_{kk'}, \quad (48)$$

$$[a_{lmk}, a_{l'm'k'}] = [a^{\dagger}_{lmk}, a^{\dagger}_{l'm'k'}] = 0. \quad (49)$$

The Hamiltonian operator for the confined bulklike LO phonon becomes

$$H_{\mathrm{LO}} = \sum_{lmk}\hbar\omega_{\mathrm{LO}}(a^{\dagger}_{lmk}a_{lmk} + \tfrac{1}{2}). \quad (50)$$

The electric potential can be expanded as

$$\phi_{\mathrm{LO}} = \sum_{lmk}\left(\frac{\hbar}{\omega_{\mathrm{LO}}}\right)^{\frac{1}{2}}(a_{lmk}\phi^{\pm}_{lmk} + \mathrm{h.c}). \quad (51)$$

The Fröhlich Hamiltonian between the electron and the confined bulklike LO phonon can then be written as

$$H_{\mathrm{e-LO}} = -e\phi_{\mathrm{LO}} = -\sum_{lmk}(\Gamma_{lmk}a^{\dagger}_{lmk}\phi^{\pm}_{lmk} + \mathrm{h.c}), \quad (52)$$

where

$$\Gamma^2_{lmk} = \frac{16\pi\hbar\omega_{\mathrm{LO}}e^2}{L_z[(l^2+m^2)\pi^2+k^2a^2]}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right). \quad (53)$$

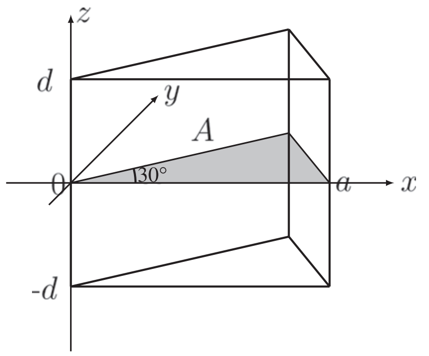

Figure 3. The geometry of the HETQD.

3. The confined bulklike LO phonon modes of the HETQD and HETQW

By the theoretical scheme of the IRTQD and IRTQW, we can derive the confined bulklike LO phonon modes and the corresponding Fröhlich electron–phonon interaction Hamiltonian of the HETQD and HETQW.

3.1. The confined bulklike LO phonon modes of the HETQD

We consider an HETQD (see figure 3) of a polar semiconductor placed in a vacuum. The height and hypotenuse of the HETQD cross section are $2d$ and a, respectively. The dielectric constant is assumed to be isotropic. Similar to the procedure for the IRTQD, the electric potential $\phi(\mathbf{r})$ can be written as

$$\phi(\mathbf{r}) = \Psi(x, y) f(z), \tag{54}$$

where $f(z)$ are equations (11) and (12). However, the HETQD cross section function $\Psi(x, y)$ is not solvable by the separation of variables. As a matter of fact, the cross section function problem is similar to the quantum mechanical problem of a particle in an hemi-equilateral triangle (billiard). On the other hand, the hemi-equilateral triangle can be obtained by subdividing the equilateral triangle along an altitude. Because these eigenfunctions of the equilateral triangle can be decomposed into a symmetric part and an antisymmetric part, the eigenfunctions of the hemi-equilateral triangle are deduced by simply restricting the antisymmetric modes of the equilateral triangle to this domain. The eigenfunctions of the hemi-equilateral triangle can be written as $\Psi_{lm}(x, y)$ [30, 32, 34, 35].

$$\begin{aligned}\Psi_{lm}(x, y) = {} & \sin\left(\frac{\sqrt{3}\pi m}{A}x\right)\sin\left[\frac{(2l+m)\pi}{A}y\right] \\ & - \sin\left(\frac{\sqrt{3}\pi l}{A}x\right)\sin\left[\frac{(2m+l)\pi}{A}y\right] \\ & + \sin\left[\frac{\sqrt{3}\pi(l+m)}{A}x\right]\sin\left[\frac{(l-m)\pi}{A}y\right],\end{aligned} \tag{55}$$

where $A = \sqrt{3}a/2$ is the altitude of the equilateral triangle. $m = 1/3, 2/3, 1, 4/3, 5/3, \ldots, l = m+1, m+2, \ldots$.

So, the eigenfunctions of the confined bulklike LO phonons can be chosen as

$$\phi^S_{lmn} = \begin{cases} C_{lmn}\Psi_{lm}(x, y) f^S(z) & \text{in HETQD,} \\ 0 & \text{otherwise,} \end{cases} \tag{56}$$

for $n = 1, 3, 5, \ldots$, and

$$\phi^A_{lmn} = \begin{cases} C_{lmn}\Psi_{lm}(x, y) f^A(z) & \text{in HETQD,} \\ 0 & \text{otherwise,} \end{cases} \tag{57}$$

for $n = 2, 4, 6, \ldots$.

The polarization vectors for the confined bulklike LO mode are calculated by considering equations (2) and (1) and the condition $\varepsilon = 0$. We get

$$\mathbf{P}^\sigma_{lmn} = \frac{1}{4\pi}\nabla\phi^\sigma_{lmn}, \qquad \sigma = S, A. \tag{58}$$

The confined bulklike LO polarization vectors from equation (58) form an orthonormal set:

$$\int \mathbf{P}^{\sigma'*}_{l'm'n'} \cdot \mathbf{P}^\sigma_{lmn}\,\mathrm{d}^3r = \frac{\sqrt{3}[16(l^2+m^2+lm)d^2+n^2A^2]}{512d} \times \delta_{\sigma\sigma'}\delta_{ll'}\delta_{mm'}\delta_{nn'}. \tag{59}$$

If we choose C_{lmn} to be

$$\begin{aligned}C^2_{lmn} &= \frac{256d}{\sqrt{3}n_p\mu[16(l^2+m^2+lm)d^2+n^2A^2]}\left(\frac{n_pe}{1+\frac{8}{3}\pi n_p\alpha}\right)^2 \\ &= \frac{64d\omega^2_{\mathrm{LO}}}{\sqrt{3}\pi[16(l^2+m^2+lm)d^2+n^2A^2]}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right),\end{aligned} \tag{60}$$

then the confined bulklike LO polarization vectors may form an orthonormal and complete set. We can express the polarization field $\mathbf{P}$ in terms of the complete set of orthonormal polarization modes $\mathbf{P}^\sigma_{lmn}$

$$\mathbf{P} = \sum_{lmn}\left(\frac{\hbar}{\omega_{\mathrm{LO}}}\right)^{\frac{1}{2}}(a^\dagger_{lmn}+a_{lmn})\mathbf{P}_{lmn}, \tag{61}$$

$$\dot{\mathbf{P}} = -\mathrm{i}\sum_{lmn}(\hbar\omega_{\mathrm{LO}})^{\frac{1}{2}}(a^\dagger_{lmn}-a_{lmn})\mathbf{P}_{lmn}, \tag{62}$$

where $\mathbf{P}$ and $\dot{\mathbf{P}}$ are now quantum field operators. $a^\dagger_{lmn}$ and a_{lmn} are creation and annihilation operators for the confined bulklike LO phonon of the (l, m, n)th mode. They satisfy the boson commutation relation (equations (36) and (37)).

The Hamiltonian operator for the confined bulklike LO phonon becomes

$$H_{\mathrm{LO}} = \sum_{lmn}\hbar\omega_{\mathrm{LO}}(a^\dagger_{lmn}a_{lmn}+\tfrac{1}{2}). \tag{63}$$

The electric potential can be expanded as

$$\phi_{\mathrm{LO}} = \sum_{lmn}\left(\frac{\hbar}{\omega_{\mathrm{LO}}}\right)^{\frac{1}{2}}(a_{lmn}\phi^\sigma_{lmn}+\mathrm{h.c}). \tag{64}$$

The Fröhlich Hamiltonian between the electron and the confined bulklike LO phonon can then be written as

$$H_{\mathrm{e-LO}} = -e\phi_{\mathrm{LO}} = -\sum_{lmn}(\Gamma_{lmn}a^\dagger_{lmn}\phi^\sigma_{lmn}+\mathrm{h.c}), \tag{65}$$

where

$$\Gamma^2_{lmn} = \frac{64de^2\hbar\omega_{\mathrm{LO}}}{\sqrt{3}\pi[16(l^2+m^2+lm)d^2+n^2A^2]}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right). \tag{66}$$

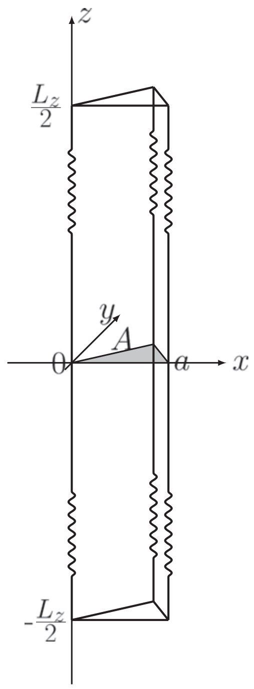

Figure 4. The geometry of the HETQW.

3.2. The confined bulklike LO phonon modes of the HETQW

Since the HETQW (see figure 4) is translationlly invariant in the z direction, the eigenfunctions of the confined bulklike LO phonons can be chosen as

$$\phi_{lmk} = \begin{cases} C_{lmk}\Psi_{lm}(x,y)\mathrm{e}^{\mathrm{i}kz} & \text{in HETQW,} \\ 0 & \text{otherwise,} \end{cases} \quad (67)$$

where k is the phonon wavevector in the z direction. The polarization vectors for the confined bulklike LO mode are

$$\mathbf{P}_{lmk} = \frac{1}{4\pi}\nabla\phi_{lmk}. \quad (68)$$

The confined bulklike LO polarization vectors form an orthonormal and complete set

$$\int 2n_p\mu\left(\frac{1+\frac{8}{3}\pi n_p\alpha}{n_p e}\right)^2 \mathbf{P}^*_{l'm'k'}\cdot\mathbf{P}_{lmk}\,\mathrm{d}^3r = \delta_{ll'}\delta_{mm'}\delta_{kk'}, \quad (69)$$

$$C^2_{lmk} = \frac{64\pi^2}{\sqrt{3}L_z n_p\mu[4(l^2+m^2+lm)\pi^2+k^2A^2]}\left(\frac{n_p e}{1+\frac{8}{3}\pi n_p\alpha}\right)^2$$
$$= \frac{16\pi\omega^2_{\mathrm{LO}}}{\sqrt{3}L_z[4(l^2+m^2+lm)\pi^2+k^2A^2]}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right), \quad (70)$$

where the L_z is the length of the HETQW.

The polarization field $\mathbf{P}$ can be expressed in terms of the complete set of orthonormal polarization modes $\mathbf{P}_{lmk}$

$$\mathbf{P} = \sum_{lmk}\left(\frac{\hbar}{\omega_{\mathrm{LO}}}\right)^{\frac{1}{2}}(a^\dagger_{lmk}+a_{lmk})\mathbf{P}_{lmk}, \quad (71)$$

$$\dot{\mathbf{P}} = -\mathrm{i}\sum_{lmk}(\hbar\omega_{\mathrm{LO}})^{\frac{1}{2}}(a^\dagger_{lmk}-a_{lmk})\mathbf{P}_{lmk}, \quad (72)$$

where $\mathbf{P}$ and $\dot{\mathbf{P}}$ are now quantum field operators. $a^\dagger_{lmk}$ and a_{lmk} are creation and annihilation operators for the confined bulklike LO phonon of the (l, m, k)th mode. They satisfy the boson commutation relation (equations (48) and (49)).

The Hamiltonian operator for the confined bulklike LO phonon becomes

$$H_{\mathrm{LO}} = \sum_{lmk}\hbar\omega_{\mathrm{LO}}(a^\dagger_{lmk}a_{lmk}+\tfrac{1}{2}). \quad (73)$$

The electric potential can be expanded as

$$\phi_{\mathrm{LO}} = \sum_{lmk}\left(\frac{\hbar}{\omega_{\mathrm{LO}}}\right)^{\frac{1}{2}}(a_{lmk}\phi_{lmk}+\mathrm{h.c}). \quad (74)$$

The Fröhlich Hamiltonian between the electron and the confined bulklike LO phonon can then be written as

$$H_{\mathrm{e-LO}} = -e\phi_{\mathrm{LO}} = -\sum_{lmk}(\Gamma_{lmk}a^\dagger_{lmk}\phi_{lmk}+\mathrm{h.c}), \quad (75)$$

where

$$\Gamma^2_{lmk} = \frac{16\pi e^2\hbar\omega_{\mathrm{LO}}}{\sqrt{3}L_z[4(l^2+m^2+lm)\pi^2+k^2A^2]}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right). \quad (76)$$

4. Summary and discussion

In this paper, we derived the exact formulations for the confined bulklike LO phonon modes, the Hamiltonian operators for the confined bulklike LO phonon and the Fröhlich Hamiltonian between the electron and the confined bulklike LO phonon in the isosceles right triangular (45°–45°–90°) quantum dot (wire) and the hemi-equilateral triangular (30°–60°–90°) quantum dot (wire). This is a starting point for the study of the polaron effect, bound polaronic effect, exciton–phonon effect, and other phonon-assisted physical processes in triangular quantum systems. For example, with the Fermi golden rule, we can use the formulations to study the electron–LO–phonon scattering rates.

As we know, we did not treat the second solution (equation (6)) in this paper, which would give the surface optical phonon modes of the isosceles right triangular quantum dot (wire) and hemi-equilateral triangular quantum dot (wire). On the other hand, if we consider the case of the isosceles right triangular quantum dot (wire) and hemi-equilateral triangular quantum dot (wire) with a finite barrier, such as these quantum dots and quantum wires surrounded by other polar semiconductors, we can deduce the interface phonon modes of these quantum dots and quantum wires. All these are part of a future research project. It is well known that the ability to model the phonon modes in dimensionally confined structures has been the basis for efforts to design nanostructures such that the resulting carrier and phonon states are tailored to yield dissipative and scattering mechanisms different from those of the corresponding bulk structures [36]. We hope these results will stimulate the study of the influence of phonons on physical properties in quantum dot and quantum wire systems of complex shapes.

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