Optical-phonon modes of circular quantum wires

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The optical-phonon modes of a circular wire are studied by means of the generalized Born-Huang equation. Its eigensolutions are found to be confined bulk and interface modes for almost all wave vectors parallel to the wire axis. At particular wave vectors hybridization of the two mode branches occurs. The eigenfrequencies and displacement eigenfields are derived for confined and interface modes. Three branches of confined modes exist, two TO and one LO. For modes confined to the wire the radial wave numbers are quantized, and determined by the zeros of Bessel functions of the first kind and of their derivatives. The twofold TO degeneracy is removed from reasons of symmetry. The displacement fields may be understood in terms of superpositions of linearly polarized plane waves with wave vectors forming a cone around the wire axis. For modes confined to the surroundings of the wire radial wave vectors remain continuous. Two types of interface modes are found. The dispersion of their frequencies with wave-vector components parallel to the wire is given in terms of modified Bessel functions. The same dispersion relations are obtained from electrostatic matching conditions. The Fröhlich interaction is studied for confined LO and interface modes. The corresponding interaction Hamiltonians are given in explicitly quantized form.

I. INTRODUCTION

Optical-phonon modes of layered structures like semiconductor superlattices and quantum wells have been extensively studied during the past.[1-11] Recently, by lateral structuring after growth or by applying particular growth techniques, some laboratories were able to create systems with an artificial microstructure in two or three dimensions.[12,13] Examples are single quantum wires and dots as well as arrays of such structures. Although the material quality and interface perfection do not yet reach those of thin layers, confinement effects of electron states have been observed.[14] Similar effects are expected for optical-phonon modes of wires and dots. In addition, interface modes should occur, and hybridization should take place of the two mode branches at certain wave vectors. Experimental evidence for phonon confinement was found by Fasol *et al.*[15] and for surface phonons by Watt *et al.*[16] Theoretically, optical-phonon modes of wires were treated by various authors by means of macroscopic[17-21] or microscopic[22,23] calculations. Stroscio *et al.*[17,18] considered rectangular wires. Besides confined LO modes, surface modes were calculated. Constantinou and Ridley[19,20] treated circular wires, and also considered LO and interface modes only. Knipp and Reinecke developed a method for dealing with interface modes of arbitrarily shaped wires and applied it to the elliptical and rectangular cases.[21] In microscopic calculations[22,23] rectangular wires were considered. Modes located at the corners were reported by Ren and Chang,[22] and hybridization effects were stressed by Zhu.[23]

In the present paper we will develop a complete macroscopic theory of optical-phonon modes of quantum wires which includes LO *and* TO confined modes as well as interface modes. The Fröhlich interaction Hamiltonians will be given in explicitly quantized form for both confined LO and interface modes.

Our analysis relies on the dispersive dielectric continuum (DCC) theory of optical-phonon modes of heterostructures developed in Ref. 24. In this approach the relative ionic displacement field is governed by a generalized Born-Huang equation which accounts for the dispersive elastic forces by means of spatial derivatives up to second order. The accompanying electric field is expressed in terms of the displacements by using rigorous macroscopic relations. In this way the generalized Born-Huang equation becomes a macroscopic eigenvalue problem. The operator of this equation represents the macroscopic counterpart of the microscopic dynamical operator of lattice theory. As it holds for the latter, the macroscopic dynamical operator has to be hermetic. It turns out that for this property to be valid, the displacement eigenfields must be either free of bulk and sheet vortices (LO confined modes), or free of bulk and sheet sources (TO confined modes), or must have neither bulk sources nor bulk vortices (Fuchs-Kliewer modes). The Hermiticity condition determines the eigensolutions of the macroscopic dynamical operator uniquely. There is no freedom for the displacement eigenfields to be adjusted to any particular boundary conditions at the interfaces; the boundary behavior follows automatically, just as in microscopic theory. It agrees with macroscopic electrodynamics, but does not correspond to any particular mechanical boundary conditions. This is consistent with the fact that macroscopic mechanics, unlike macroscopic electrodynamics, does not impose any restrictions on the *relative* ionic displacements. The field which enters the elastic continuum theory is that of the *center of mass* of the ions of a unit cell rather than that of their relative displacements. Setting mechanical boundary conditions leads either to the loss of Hermiticity of the dynamical operator—then the conditions are poor—or it does not affect Hermiticity, in

which case the conditions are needless. This applies to macroscopic theories which include spatial derivatives of the relative displacement field up to second order. The role of mechanical boundary conditions changes if higher-order derivatives are taken into account, either in the elastic or the electric forces.[8,11,25,26] Then one may put mechanical boundary conditions without necessarily losing Hermiticity, and achieve better agreement with microscopic theory. This implies, however, numerical calculations of eigensolutions, i.e., the loss of the advantage of macroscopic theories which provide explicit analytical expressions for eigenfrequencies, displacement eigenvectors, and Fröhlich interaction Hamiltonians.

Of course, there are limitations of the DDC theory. For instance, this theory fails to give unique answers if modes of different branches are degenerate at certain wave vectors $\mathbf{Q}_c$. For GaAs-AlAs superlattices such degeneracy takes place between GaAs confined modes and GaAs-like interface modes. Although the DCC theory *does* indicate that confined and interface mode displacement fields will hybridize at the degeneracy points $\mathbf{Q}_c$, it neither specifies the particular form of hybridization nor removes the frequency degeneracy. The reason for this is the lack of any specific short-range forces across the interfaces. If one includes such forces in the DCC model, finite splittings and definite hybrid solutions may be derived by means of perturbation theory. Hybridization represents an interesting theoretical phenomenon, but it does not result in dramatic changes of eigenfrequencies and eigenvectors, if treated correctly. As microscopic calculations by Ren, Chu, and Chang[7] for $(GaAs)_7$-$(AlAs)_7$ superlattices demonstrate, its neglect may be a reasonable approximation for almost all wave vectors. This is not surprising since perturbations of short-range interactions at interfaces should only weakly affect *collective* lattice excitations like confined or interface modes.

Another noticeable error of the DCC theory arises in the case of LO displacement fields of GaAs-AlAs superlattices with wave vector $\mathbf{Q}=(\mathbf{q}=\mathbf{0}, k\rightarrow 0)$ approaching zero parallel to the superlattice (SL) axis. While microscopic displacements tend smoothly to zero at the interfaces in this case,[27] macroscopic displacements decay suddenly.[24] In the DDC theory this happens independently of wave vector, i.e., also for $\mathbf{Q}=(\mathbf{q}\rightarrow\mathbf{0},0)$. For such $\mathbf{Q}$ the microscopic theory yields almost sudden displacement changes at interfaces,[27] just as predicted macroscopically. The observed alteration of microscopic confined LO modes with k means a wave-vector dispersion which may only occur if the confinement is not complete, as it happens obviously in microscopic theory. In macroscopic theory, on the contrary, confinement is perfect; thus no k dispersion may take place. The relative ionic displacement fields which apply for $(\mathbf{q},k\rightarrow 0)$ are also valid for $(\mathbf{q}\rightarrow 0,0)$. The occurrence of sudden changes of relative displacements in a continuum theory is neither unexpected nor does it indicate any unphysical behavior. It means that finite changes of relative displacements take place on a length scale defined by the interatomic spacing. Macroscopically, this spacing is taken to be zero; thus discontinuities arise.

In summary, the dispersive dielectric continuum theory represents the simplest complete macroscopic theory of the optical-phonon modes of heterostructures. It avoids the failure of the nondispersive dielectric continuum model in determining unique displacement eigenfields of confined modes.[8] Without dispersion these modes are degenerate, and any linear combination of eigenfields is allowed. Thus the macroscopic theory of optical-phonon modes of heterostructures cannot be based on the nondispersive dielectric continuum model; dispersion has to be included. The dispersive dielectric continuum theory reproduces well all main features of polar optical-phonon modes of heterostructures. It is qualitatively correct without any exception. Quantitative deviations from the true microscopic results arise from the continuum character of the theory. They are small in most cases, and remarkable but still tolerable in a few other cases. The theory yields confined modes and interface modes, and indicates the $\mathbf{Q}$ vectors where hybridization of both may take place. Analytical expressions are obtained for eigenfrequencies and eigenfields in the entire mode spectrum. The orthogonality and completeness of modes may be demonstrated explicitly.[24] Eigenfrequencies of confined modes are close to microscopic values, and the dispersion of interface modes is exactly that by Fuchs and Kliewer[24]—also in good agreement with microscopic theory. Electrostatic potentials are close to those from microscopic calculations[27] for all modes and wave vectors. Thus reliable Fröhlich interaction Hamiltonians are provided both for confined LO and interface modes. The displacement fields of all modes exhibit the correct symmetry, provided the assignment of microscopic and macroscopic modes is done properly, i.e., according to the number of nodes. The actual displacements of confined and interface modes are in reasonable agreement with those from microscopic theory, although the changes at interfaces are less steep in microscopic than in macroscopic theory. This discrepancy represents an artifact of any strict continuum theory since here the interatomic spacings are set equal to zero.

Originally, the dispersive dielectric continuum theory has been developed in the case of superlattices. In the present paper we will use it in order to investigate quantum wires. We consider a single circular wire since the latter represents the simplest theoretical case from which one may proceed in order to understand rectangular wires and arrays also. The paper is organized as follows: In Sec. II we set up the eigenvalue problem. Its solutions are classified in Sec. III. Confined modes are treated in Sec. IV, and interface modes in Sec. V. The electron-phonon interaction is considered in Sec. VI. Section VII concludes the paper.

II. THE EIGENVALUE PROBLEM

We take an infinite wire, made of a certain zincblende-type material (1). The infinite space around it is assumed to be filled with another zincblende-type material (2) or vacuum (see Fig. 1). The macroscopic theory of optical-phonon modes deals with the mechanical displacement field $\mathbf{u}(\mathbf{x},t)$. In the limit of long wavelengths, $\mathbf{u}(\mathbf{x},t)$ turns into the relative displacements of the two

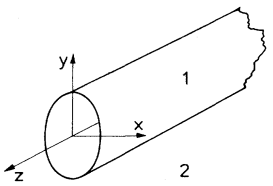

FIG. 1. Geometry of a circular quantum wire.

atoms of a unit cell at a lattice position $\mathbf{x}$ which is thought to be continuously varying.[24] The mechanical displacement field results in an electric polarization field $\mathbf{P}(\mathbf{x},t)$ given by

$$\mathbf{P}(\mathbf{x},t)=N(\mathbf{x})e^*(\mathbf{x})\mathbf{u}(\mathbf{x},t)\ , \tag{1}$$

where $e^*(\mathbf{x})$ means the dynamical charge and $N(\mathbf{x})$ the density of unit cells of the material at position $\mathbf{x}$. For $\mathbf{x}$ in material j, $j=1,2$, we set $e^*(\mathbf{x})=e_j^*$ and $N(\mathbf{x})=N_j$. The same notation scheme will also be applied to other material parameters. The polarization field $\mathbf{P}(\mathbf{x},t)$ is connected with an electric field $\mathbf{E}(\mathbf{x},t)$ and a dielectric displacement field $\mathbf{D}(\mathbf{x},t)$. The four quantities $\mathbf{u}(\mathbf{x},t)$, $\mathbf{P}(\mathbf{x},t)$, $\mathbf{E}(\mathbf{x},t)$, and $\mathbf{D}(\mathbf{x},t)$ are governed by the coupled set of Newton's and Maxwell's equations. With $\mathbf{u}(\mathbf{x})$, $\mathbf{P}(x)$, $\mathbf{E}(\mathbf{x})$, and $\mathbf{D}(\mathbf{x})$ being the time Fourier transforms of these fields, Newton's equation reads[24,25,28]

$$\{\omega_T^2(\mathbf{x})-c_T^2(\mathbf{x})\nabla\times\nabla+c_L^2(\mathbf{x})\nabla\nabla\cdot-\omega^2\}\mathbf{u}(\mathbf{x}) -[e^*(\mathbf{x})/M(\mathbf{x})]\mathbf{E}(\mathbf{x})=0\ . \tag{2}$$

Here, $\omega_T(\mathbf{x})$ means the TO frequency and $M(\mathbf{x})$ the reduced mass of the two atoms of a unit cell; $c_T(\mathbf{x}),c_L(\mathbf{x})$ denote certain velocities. The latter describe elastic (or long-range mechanical) forces being responsible for the wave-vector dispersion of optical phonons. Equation (2) holds in the entire space with the exclusion of the wire boundary. In particular, it cannot be applied across this boundary in order to prove the continuity of the displacement fields and their first derivatives there. These fields may have discontinuities at the wire interface. This does not mean, however, that infinite elastic forces will occur since Eq. (2) does not hold there. It rather indicates the transformation of elastic forces into short-range mechanical forces.[24] If, in contrast, acoustic modes of long wavelengths are considered, the mechanical displacement field which enters is that of the *center of mass* of the two atoms of a unit cell. No short-range forces exist, and the second derivatives of the displacement field describe elastic forces everywhere. An equation of motion analogous to Eq. (2) holds also at the wire interface. Thus the continuity of the acoustical displacement field and of certain components of its first derivatives may also be derived there. From a microscopic point of view, the discontinuities of the *relative* displacement field $\mathbf{u}$ mean that finite changes take place on a short-range distance. Macroscopically, the short-range scale is taken to be zero; thus finite short-range changes of $\mathbf{u}$ become abrupt.

For the electric-field vectors $\mathbf{P}(\mathbf{x}),\mathbf{E}(\mathbf{x}),\mathbf{D}(\mathbf{x})$, one may use equations which follow from Maxwell's theory with the neglect of retardation (or polariton) effects. This approximation breaks down for phonon wave numbers Q at the crossings of phonon and photon dispersion curves, i.e., at $Q=\omega_T/c$, with c being the light velocity. Such wave numbers are extremely small, even much smaller than wave numbers of phonons excited in common Raman experiments which are of the order of magnitude of photon wave numbers and, therefore, small compared to the extension of the first Brillouin zone (BZ). This means that for phonons which show up in common Raman experiments, the neglect of polariton effects is well justified. The same applies to the majority of phonons which take part in free-carrier scattering. Thus Maxwell's equations read approximately

$$\nabla\times\mathbf{E}(\mathbf{x})=0\ , \tag{3}$$

$$\nabla\cdot\mathbf{D}(\mathbf{x})=0\ . \tag{4}$$

In addition, one has

$$4\pi\mathbf{P}(\mathbf{x})=\mathbf{D}(\mathbf{x})-\epsilon_\infty(\mathbf{x})\mathbf{E}(\mathbf{x})\ . \tag{5}$$

Here, $\epsilon_\infty(\mathbf{x})$ means the purely electronic part of the dielectric function. Equations (1), (3), (4), and (5) may be used in order to express $\mathbf{E}(\mathbf{x})$ as a certain linear functional $\hat{E}[\mathbf{u}(\mathbf{x})]$ of the relative displacement field $\mathbf{u}(\mathbf{x})$. Later we will determine $\hat{E}$ explicitly. Here its existence suffices. It means that (2) represents an eigenvalue equation for ω^2 and $\mathbf{u}$. Optical-phonon frequencies and displacement fields are the solutions of this equation—more strictly, solutions which obey the following additional requirements.

(i) The eigenfields $\mathbf{u}$ are normalized. We use periodic boundary conditions with respect to a certain periodicity length Ga parallel to the wire axis which is taken parallel to z, i.e., we set

$$\mathbf{u}(\mathbf{x}+Ga\,\mathbf{e}_z)=\mathbf{u}(\mathbf{x})\ , \tag{6}$$

where G means a large integer, a the lattice constant, and $\mathbf{e}_z$ a unit vector parallel to z. Normalization is required with respect to the periodicity slab (PS), $-\infty<x<\infty$, $-\infty<y<\infty$, $0<z<Ga$. One has

$$\int_{\mathrm{PS}} d^3\mathbf{x}\,\mathbf{u}^*(\mathbf{x})\cdot\mathbf{u}(\mathbf{x})=1\ . \tag{7}$$

(ii) From physical reasons, the eigenvalues ω^2 are expected to be real; thus the operator $\tilde{D}$ of the eigenvalue problem has to be Hermitian. Apart from the wire boundary, $\tilde{D}$ is identical with the dynamical operator

$$D=\omega_T^2(\mathbf{x})-c_T^2(\mathbf{x})\nabla\times\nabla\times+c_T^2(\mathbf{x})\nabla\nabla\cdot-[e^2(\mathbf{x})/M(\mathbf{x})]\hat{E} \tag{8}$$

of Eq. (2). *On* the wire boundary, $\tilde{D}$ is not given by D. Its actual values are unknown there, but one may assume them to be finite. Then the Hermiticity condition becomes

$$\int_{\mathrm{PS}} d^3\mathbf{x}[\mathbf{w}^*\cdot D\mathbf{u}-\mathbf{u}\cdot D\mathbf{w}^*]=0\ , \tag{9}$$

with $\mathbf{u},\mathbf{w}$ being two arbitrary displacement fields. The integral in (9) extends upon a periodicity slab with the ex-

cept of the wire boundary. The exclusion of this surface does not change the value of the original Hermiticity integral since $\tilde{D}$ remains finite. The Hermiticity condition guarantees also that eigenfields of different eigenvalues are orthogonal and that a complete set of orthonormalized vector fields may be formed from eigenvectors.

The dynamical operator $\tilde{D}$ exhibits full translational and rotational symmetries with respect to the wire axis. Thus its eigenvalues are highly degenerate, and the eigenfunctions of a certain eigenvalue may be subjected to an arbitrary unitary transformation. One may remove this arbitrariness by demanding the eigenfunctions to form basis sets of irreducible representations of the translational and rotational symmetry groups of $\tilde{D}$. These representations are one dimensional and are characterized by a wave vector q for the translational group and an integer

$$m=0,\pm1,\pm2,\ldots,\pm\infty$$

for the rotational group. In order to fulfill the periodicity condition (6), the wave number q has to be taken as $(2\pi/Ga)l$, with l being an integer varying between $-\frac{1}{2}G$ and $\frac{1}{2}G-1$. In general, eigenfrequencies and eigenfields for different values of q,m will differ. For given q,m, still different eigensolutions exist corresponding to different phonon branches t. We write ω_{tmq} and $\mathbf{u}_{tmq}(\mathbf{x})$. By definition, the eigenfields $\mathbf{u}_{tmq}(\mathbf{x})$ are of the general form

$$\mathbf{u}_{tmq}(\mathbf{x})=\mathbf{u}_{tmq}(r)e^{i(m\varphi+qz)}\ , \tag{10}$$

where r,φ,z are the cylinder coordinates of $\mathbf{x}$.

III. CLASSIFICATION OF EIGENSOLUTIONS

The various optical-phonon eigenmodes of a wire may be characterized by the vanishing or nonvanishing of the sources and vortices of their displacement eigenfields $\mathbf{u}_{smq}(\mathbf{x})$. For a superlattice this has been demonstrated in Ref. 24. Here we apply the analysis developed in Ref. 24 to a wire. Conditions for sources $\nabla\cdot\mathbf{u}_{tmq}$ and vortices $\nabla\times\mathbf{u}_{tmq}$ follow by applying the operators $\nabla\cdot$ and $\nabla\times$ to the eigenvalue equation (2), using simultaneously the electrodynamic equations (1), (3), (4), and (5). The latter result in

$$-[e^*(\mathbf{x})/M(\mathbf{x})]\nabla\cdot\mathbf{E}=\omega_p^2(\mathbf{x})\nabla\cdot\mathbf{u}\ , \tag{11}$$

with

$$\omega_p^2(\mathbf{x})=[4\pi e^{*2}(\mathbf{x})N(\mathbf{x})]/[\epsilon_\infty(\mathbf{x})M(\mathbf{x})]$$

being the lattice plasmon frequency. With the except of the wire boundary at $r=R$, one gets

$$[\omega_{1T}^2+c_{1T}^2\Delta-\omega_{tmq}^2]\nabla\times\mathbf{u}_{tmq}(\mathbf{x})=0,\quad \mathbf{x}\text{ in }1 \tag{12a}$$

$$[\omega_{2T}^2+c_{2T}^2\Delta-\omega_{tmq}^2]\nabla\times\mathbf{u}_{tmq}(\mathbf{x})=0,\quad \mathbf{x}\text{ in }2 \tag{12b}$$

$$[\omega_{1L}^2+c_{1L}^2\Delta-\omega_{tmq}^2]\nabla\cdot\mathbf{u}_{tmq}(\mathbf{x})=0,\quad \mathbf{x}\text{ in }1 \tag{13a}$$

$$[\omega_{2L}^2+c_{2L}^2\Delta-\omega_{tmq}^2]\nabla\cdot\mathbf{u}_{tmq}(\mathbf{x})=0,\quad \mathbf{x}\text{ in}2\ . \tag{13b}$$

Here the LO phonon frequencies ω_{jL} have been introduced by means of the relation $\omega_{jL}^2=\omega_{jT}^2+\omega_{jp}^2$, $j=1,2$. Equations (12) and (13) mean that $\nabla\times\mathbf{u}_{tmq}$ and $\nabla\cdot\mathbf{u}_{tmq}$ must either vanish or be eigenfunctions of the Laplacian operator Δ. In both cases, one may write

$$\Delta\nabla\times\mathbf{u}_{tmq}=-(q^2+K_{tTm}^2)\nabla\times\mathbf{u}_{tmq}\ , \tag{14}$$

$$\Delta\nabla\cdot\mathbf{u}_{tmq}=-(q^2+K_{tLm}^2)\nabla\cdot\mathbf{u}_{tmq}\ , \tag{15}$$

with $-(q^2+K_{tTm}^2)$ and $-(q^2+K_{tLm}^2)$ being the eigenvalues. By combining equations (12) and (13) with (14) and (15), one obtains the set of equations

$$[\omega_{1T}^2-c_{1T}^2(q^2+K_{tTm}^2)-\omega_{tmq}^2]\nabla\times\mathbf{u}_{tmq}=0,\quad \mathbf{x}\text{ in }1 \tag{16a}$$

$$[\omega_{2T}^2-c_{2T}^2(q^2+K_{tTm}^2)-\omega_{tmq}^2]\nabla\times\mathbf{u}_{tmq}=0,\quad \mathbf{x}\text{ in }2 \tag{16b}$$

$$[\omega_{1L}^2-c_{1L}^2(q^2+K_{tLm}^2)-\omega_{tmq}^2]\nabla\cdot\mathbf{u}_{tmq}=0,\quad \mathbf{x}\text{ in }1 \tag{17a}$$

$$[\omega_{2L}^2-c_{2L}^2(q^2+K_{tLm}^2)-\omega_{tmq}^2]\nabla\cdot\mathbf{u}_{tmq}=0,\quad \mathbf{x}\text{ in }2\ . \tag{17b}$$

For a certain eigensolution ω_{tmq}^2 and $\mathbf{u}_{tmq}$, these equations have to be fulfilled simultaneously. We assume the four bulk dispersion curves

$$\omega_{jT/LQ}^2=\omega_{jT/L}^2-c_{jT/L}^2Q^2 \tag{18}$$

to be free of any overlap, i.e.,

$$\omega_{1TQ}\neq\omega_{2TQ}\neq\omega_{1LQ}\neq\omega_{2LQ} \tag{19}$$

is required for any relevant wave vector $\mathbf{Q}$ of the first bulk BZ. This means that for a certain eigenvalue ω_{tmq}, only one of the square brackets in Eqs. (16) and (17) may be equal to zero. Let it be the first one, i.e., let us assume

$$\omega_{tmQ}^2=\omega_{1T}^2-c_{1T}^2(q^2+K_{tTm}^2)\ .$$

Then $\nabla\times\mathbf{u}_{tmq}$ may differ from zero in material 1 and must vanish in material 2, while $\nabla\cdot\mathbf{u}_{tmq}$ has to be zero in both materials. The index t of this mode is set equal to $1TK$. Later we will demonstrate that $\mathbf{u}_{1TKmq}$ will be zero in material 2 by itself, i.e., $\mathbf{u}_{1TKmq}$ will be confined to material 1. It represents the material-1-like transverse confined mode of radial wave number K_{1Tm}. In a similar way, one finds three other branches of confined bulk modes being the material-2-like transverse ($t=2TK$) and the material-1- or -2-like longitudinal branches ($t=1LK,2LK$).

There is still another way of satisfying the system of equations (16) and (17). Vortices and sources of the displacement fields $\mathbf{u}_{tmq}$ may be set equal to zero in both materials. Since $\mathbf{u}_{tmq}$ may have discontinuities on the wire boundary, nonvanishing sheet vortices and sources may exist on this surface. Then $\mathbf{u}_{tmq}(\mathbf{x})$ may differ from zero despite the vanishing of bulk vortices and sources. The corresponding modes are termed "interface modes" and labeled by $t=I$. Their eigenfrequencies ω_{Imq} will differ in general from those of confined bulk modes.

The behavior of the displacement fields of confined bulk modes $\mathbf{u}_{tmq}$, $t=jT/L$, $j=1,2$, at the wire boundary follows from the Hermiticity condition (9). One finds that the normal components of the displacement fields of transverse modes are continuous, and the parallel com-

TABLE I. Classification of optical-phonon modes of a cylindrical heterostructure. IF means interface.

	1TO	2TO	1LO	2LO	I
$\nabla\times\mathbf{u}_{tmq}$ in 1	$\neq 0$	0	0	0	0
$\nabla\times\mathbf{u}_{tmq}$ in 2	0	$\neq 0$	0	0	0
$\nabla\cdot\mathbf{u}_{tmq}$ in 1	0	0	$\neq 0$	0	0
$\nabla\cdot\mathbf{u}_{tmq}$ in 2	0	0	0	$\neq 0$	0
$\nabla\times\mathbf{u}_{tmq}$ on IF	$\neq 0$	$\neq 0$	0	0	$\neq 0$
$\nabla\cdot\mathbf{u}_{tmq}$ on IF	0	0	$\neq 0$	$\neq 0$	$\neq 0$

ponents jump. For longitudinal modes the normal components jump, and the parallel components are continuous. This means that transverse confined bulk modes are free of both bulk *and* sheet sources, but have bulk and sheet vortices, while longitudinal confined bulk modes are free of bulk and sheet vortices, but have bulk and sheet sources. Table I summarizes the results of this section.

IV. CONFINED BULK MODES

LO modes

According to Sec. III, the displacement fields of confined LO modes obey the equations

$$\nabla\times\mathbf{u}_{jLKmq}=0, \quad \mathbf{x} \text{ in } 1,2 \tag{20}$$

$$\Delta\nabla\cdot\mathbf{u}_{jLKmq}=\begin{cases}-(q^2+K_{jLm}^2)\nabla\cdot\mathbf{u}_{jLKmq}, & \mathbf{x} \text{ in } j\\ 0, & \mathbf{x} \text{ in } j'\neq j\ .\end{cases} \tag{21}$$

The displacement eigenfields $\mathbf{u}_{jLKmq}$ which solve these equations are not unique. By adding an arbitrary vector field having no bulk sources and vortices, i.e., an interface mode displacement field, one obtains again a solution. However, displacement fields of eigenmodes are also governed by the eigenvalue equations (16) and (17). This causes the interface mode part to be zero provided the confined LO mode eigenfrequency ω_{1LKmq} differs from that of any interface (IF) mode eigenfrequency ω_{Imq} for the same values of m,q. Later we will see that this condition holds for almost all q, except for particular ones where the dispersion curves ω_{jLKmq} and ω_{Imq} cross. Such values of q will be excluded from the consideration which follows (see Ref. 24 for a more comprehensive discussion). Then the displacement eigenfields $\mathbf{u}_{jLKmq}$ are of the general form

$$\mathbf{u}_{jLKmq}(\mathbf{x})=C_{jLKmq}\Lambda_j(r)\mathbf{v}_{jLKmq}(r)e^{i(m\varphi+qz)}\ , \tag{22}$$

with

$$\Lambda_j(r)=[\delta_{j1}\theta(R-r)+\delta_{j2}\theta(r-R)] \tag{23}$$

expressing the confinement of modes with $j=1$ to the wire, and with $j=2$ to its surroundings, while C_{jLKmq} denotes a normalization constant. By using (22), the upper part of Eq. (21) becomes

$$\left[\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\left[K_{jLm}^2-\frac{m^2}{r^2}\right]\right]\nabla\cdot\mathbf{u}_{jLKmq}=0\ , \quad \mathbf{x} \text{ in } j\ . \tag{24}$$

Equation (24) is solved by Bessel functions $J_m(K_{jLm}r)$ and $Y_m(K_{jLm}r)$ of the first and second kind.[29,30] Since $Y_m(K_{jLm}r)$ diverges for $r\to 0$, only $J_m(K_{jLm}r)$ is allowed for $j=1$, i.e., for modes confined to the wire. One gets

$$\nabla\cdot\mathbf{u}_{1LKmq}(\mathbf{x})=c\Lambda_1(r)J_m(K_{1Lm}r)e^{i(m\varphi+qz)}\ , \tag{25a}$$

with c being an arbitrary constant. For modes confined to material 2, i.e., to the wire surroundings, any linear combinations of $J_m(K_{2Lm}r)$ and $Y_m(K_{2Lm}r)$ may be taken as solutions of Eq. (24). Thus one obtains

$$\nabla\cdot\mathbf{u}_{2LKmq}(\mathbf{x})=b\Lambda_2(r)[J_m(K_{2Lm}r)+\beta Y_m(K_{2Lm}r)]\times e^{i(m\varphi+qz)}\ , \tag{25b}$$

where b and β are certain constants.

The vortex equation (20) means that $\mathbf{u}_{jLKmq}(\mathbf{x})$ may be expressed as a gradient of a scalar function

$$\psi_{jLKmq}(r)\exp[i(m\varphi+qz)]\ ,$$

as follows:

$$\mathbf{u}_{jLKmq}(\mathbf{x})=\nabla[\psi_{jLKmq}(r)e^{i(m\varphi+qz)}], \quad \mathbf{x} \text{ in } j\ . \tag{26}$$

By using $\nabla\cdot\mathbf{u}_{1LKmq}$ from (25) and setting $c=-(K_{1Lm}^2+q^2)$, $b=-(K_{2Lm}^2+q^2)$, one arrives at the following equation for $\psi_{1LKmq}(r)$:

$$\left[\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\left[q^2+\frac{m^2}{r^2}\right]\right]\psi_{jLKmq}(r)=-(q^2+K_{jLm}^2)\begin{cases}J_m(K_{1Lm}r)\\ J_m(K_{2Lm}r)+\beta Y_m(K_{2Lm}r)\ .\end{cases} \tag{27}$$

It is solved by

$$\psi_{jLKmq}(r)=\begin{cases}J_m(K_{1Lm}r), & j=1\\ J_m(K_{2Lm}r)+\beta Y_m(K_{2Lm}r), & j=2\ .\end{cases} \tag{28}$$

This solution determines the radial part $\mathbf{v}_{jLKmq}(r)$ of $\mathbf{u}_{jLKmq}(\mathbf{x})$ from (22) by means of Eq. (26). In performing the vector operation ∇, we use the set of cylindrical unit vectors $\mathbf{e}_r,\mathbf{e}_\varphi,\mathbf{e}_z$. One gets

$$\mathbf{v}_{1LKmq}(r)=J_m'(K_{1Lm}r)\mathbf{e}_r+i\frac{m}{K_{1Lm}r}J_m(K_{1Lm}r)\mathbf{e}_\varphi+i\frac{q}{K_{1Lm}}J_m(K_{1Lm}r)\mathbf{e}_z\ , \tag{29a}$$

TABLE II. Zeros of Bessel functions $J_m(z)$ and their derivatives $J'_m(z)$.

	z_{Km}				z'_{Km}			
m	0	1	2	3	0	1	2	3
$K=1$	2.4	3.8	5.1	6.4	3.8	1.8	3.1	4.2
$K=2$	5.5	7.0	8.4	9.8	7.0	5.3	6.7	8.0
$K=3$	8.5	10.1	11.6	13.0	10.2	8.5	10.0	11.4
$K=4$	11.8	13.3	14.8	16.2	13.3	11.7	13.2	14.6

$$\mathbf{v}_{2LKmq}(r)=[J'_m(K_{2Lm}r)+\beta Y'_m(K_{2Lm}r)]\mathbf{e}_r + i\frac{m}{K_{2Lm}r}[J_m(K_{2Lm}r)+\beta Y_m(K_{2Lm}r)]\mathbf{e}_\varphi + i\frac{q}{K_{2Lm}}[J_m(K_{2Lm}r)+\beta Y_m(K_{2Lm}r)]\mathbf{e}_z \ . \tag{29b}$$

In order to fulfill the Hermiticity condition, the parallel components of $\mathbf{v}_{jLKmq}(r)$ must vanish on the wire interface. For fields within the wire, i.e., for $j=1$, this yields a condition for K_{1Lm}. It reads

$$J_m(K_{1Lm}R)=0 \ . \tag{30a}$$

This means that the radial wave number K_{1Lm} is quantized according to

$$K_{1Lm}=(z_{Km}/R), \quad K=1,2,\ldots,\infty \tag{30b}$$

where z_{Km} means the Kth zero of the Bessel function $J_m(z)$ (see Table II). Outside the wire, the vanishing of the parallel component at the interface means

$$[J_m(K_{2Lm}R)+\beta Y_m(K_{2Lm}R)]=0 \ . \tag{31}$$

Relation (31) fixes the coefficient β but does not result in a quantization of the radial wave vector K_{2Lm}. The latter remains continuous. The normalization constant C_{1LKmq} of the in-wire eigenfield $\mathbf{u}_{1LKmq}$ from Eq. (22) becomes

$$C_{1LKmq}=\frac{1}{\sqrt{\Omega}}\left[\frac{K_{1Lm}^2}{q^2+K_{1Lm}^2}\,\frac{-1}{[J_{m-1}(K_{1Lm}R)][J_{m+1}(K_{1Lm}R)]}\right]^{1/2}, \tag{32}$$

where Ω means the volume $\pi R^2 Ga$ of a periodicity part of the wire. Eigenfields $\mathbf{u}_{2LKmq}$ outside the wire are to be normalized in the sense of Dirac's δ function depending on the radial wave-number differences $K_{2Lmq}-K'_{2Lmq}$. The normalization integrals may be taken by means of formulas given in Ref. 30. This yields explicit expressions for the normalization factors C_{2LKmq}. We do not write them down here.

The eigenfrequencies ω_{jLKmq} of the longitudinal confined modes are given by

$$\omega_{jLKmq}^2=\omega_{jL}^2-c_{jL}^2(q^2+K_{jLm}^2) \ . \tag{33}$$

Since the quantized wave numbers K_{1Lm} depend on m, the degeneracy of LO frequencies which takes place for homogeneous and isotropic systems is removed in the case of a wire as long as its interior is considered. Outside the wire, the LO spectrum remains continuous. The LO mode displacement fields (29) and eigenfrequencies (33) inside the wire agree with those obtained by Constantinou and Ridley in Ref. 19.

TO modes

The displacement fields $\mathbf{u}_{jTKmq}$ of transverse confined modes obey the relations

$$\nabla\cdot\mathbf{u}_{jTKmq}(\mathbf{x})=0, \quad \mathbf{x} \text{ in } 1,2 \tag{34}$$

$$\Delta\nabla\times\mathbf{u}_{jTKmq}=\begin{cases}-(q^2+K_{jTm}^2)\nabla\times\mathbf{u}_{jTKmq}, & \mathbf{x} \text{ in } j\\ 0, & \mathbf{x} \text{ in } j'\neq j \ .\end{cases} \tag{35}$$

By using the same arguments as in the case of LO modes, one arrives at the conclusion that the general form of $\mathbf{u}_{jTKmq}(\mathbf{x})$ reads

$$\mathbf{u}_{jTKmq}(\mathbf{x})=C_{jTKmq}\Lambda_j(r)\mathbf{v}_{jTKmq}(r)e^{i(m\varphi+qz)} \ . \tag{36}$$

The radial parts $\mathbf{v}_{jTKmq}(r)$ in (36) may be determined in a similar way as in the LO case. One finds that two transverse modes exist. They will be labeled by T_s and T_p. Modes confined to the wire or to its surroundings are to be treated separately.

(i) Within the wire, one obtains

$$\mathbf{v}_{1T_sKmq}(r)=C_{1T_sKmq}\left[\frac{m}{K_{1Tsm}r}J_m(K_{1Tsm}r)\mathbf{e}_r + iJ'_m(K_{1Tsm}r)\mathbf{e}_\varphi\right], \tag{37}$$

$$\mathbf{v}_{1T_pKmq}(r)=C_{1T_pKmq}\left[J'_m(K_{1Tpm}r)\mathbf{e}_r + i\frac{m}{K_{1Tpm}r}J_m(K_{1Tpm})\mathbf{e}_\varphi - i\frac{K_{1Tpm}}{q}J_m(K_{1Tpm}r)\mathbf{e}_z\right] . \tag{38}$$

From the Hermiticity condition it follows that the normal components of transverse modes have to be continuous on the wire interface. This yields

$$J_m(K_{1Tsm}R)=0 , \tag{39a}$$

$$J'_m(K_{1Tpm}R)=0 . \tag{39b}$$

The quantization condition for K_{1Tsm} is the same as that for LO modes. Thus one obtains

$$K_{1Tsm}=K_{1Lm}=(z_{Km}/R) . \tag{40}$$

For K_{1Tpm} one has

$$K_{1Tpm}=(z'_{Km}/R) , \tag{41}$$

where z'_{Km} means the Kth zero of $J'_m(z)$ ($K=1,2,\ldots,\infty$) (see Table II). The normalization factors of the corresponding eigenfields $\mathbf{u}_{1T_{s/p}Kmq}$ in (36) are given by

$$C_{1T_sKmq}=\frac{1}{\sqrt{\Omega}}\frac{1}{[-J_{m-1}(K_{1Tsm}R)J_{m+1}(K_{1Tsm}R)]^{1/2}} , \tag{42}$$

$$C_{1T_pKmq}=\frac{1}{\sqrt{\Omega}}\left[\frac{q^2}{q^2+K^2_{1Tpm}}\frac{1}{J^2_m(K_{1Tpm}R)-J_{m-1}(K_{1Tpm}R)J_{m+1}(K_{1Tpm}R)}\right]^{1/2} . \tag{43}$$

The quantized wave numbers $K_{1Ts/pmq}$ result in eigenfrequencies $\omega_{1Ts/pKmq}$ of transverse confined modes given by the relation

$$\omega^2_{1Ts/pKmq}=\omega^2_{1T}-c^2_{1T}(q^2+K^2_{1Ts/pm}) . \tag{44}$$

Due to the different values of K_{1Tsm} and K_{1Tpm}, the degeneracy of the two transverse modes which takes place for homogeneous isotropic materials is removed in the case of a wire for modes confined to its interior. Furthermore, since K_{1Tsm} and K_{1Tpm} depend on m, there is also no mode degeneracy with respect to m. This behavior may be easily understood. As shown in the Appendix, confined bulk modes of branch t represent superpositions of linearly polarized plane waves of polarization $\mathbf{e}_t(\varphi')$ and wave vectors forming a cone around the wire axis (see Fig. 2). The two polarization vectors $\mathbf{e}_{T_s}(\varphi')$ and $\mathbf{e}_{T_p}(\varphi')$ in Fig. 2 which give rise to T_s and T_p confined modes have nonequivalent directions with respect to the wire axis, i.e., no symmetry transformation of the wire exists which transforms $\mathbf{e}_{T_s}(\varphi')$ into $\mathbf{e}_{T_p}(\varphi')$. For $q\to 0$, in particular, $\mathbf{e}_{T_s}(\varphi')$ becomes tangential to the wire surface and perpendicular to the wire axis, while $\mathbf{e}_{T_p}(\varphi')$ becomes parallel to the wire axis. In the same limit, $\mathbf{e}_L(\varphi')$, giving rise to LO confined modes, becomes perpendicular to the wire interface.

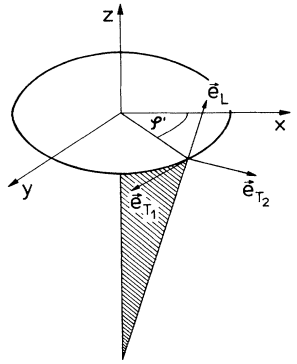

FIG. 2. Construction of eigenmodes with cylindrical symmetry.

The m degeneracy which holds in the case of a homogeneous isotropic material follows from the full spherical symmetry of the system. Its removal in the case of a wire is due to the transition from spherical to axial symmetry.

(ii) Outside the wire, no radial wave-vector quantization takes place, as in the case of LO modes. The radial parts of displacement eigenfields may be obtained from expressions (37) and (38) by replacing $J_m(K_{1Ts/pm}r)$ there by

$$[J_m(K_{2Ts/pm}r)+\beta Y_m(K_{2Ts/pm}r)] .$$

The factor β follows from the condition that the normal components of the displacement fields must vanish at the wire interface. This yields

$$[J_m(K_{2Tsm}R)+\beta Y_m(K_{2Tsm}R)]=0 , \tag{45}$$

$$[J'_m(K_{2Tpm}R)+\beta Y'_m(K_{2Tpm}R)]=0 . \tag{46}$$

Orthogonality. Eigenfields of different confined modes are orthogonal. This may be shown explicitly by using the above-derived expressions for $\mathbf{u}_{jbKmq}$, $b=L,T_1,T_2$. One has

$$(\mathbf{u}_{j'b'K'm'q'}|\mathbf{u}_{jbKmq})=\delta_{j'j}\delta_{b'b}\delta_{K'K}\delta_{m'm}\delta_{q'q} , \tag{47}$$

where $\delta_{K'K}$ has to be replaced by $\delta(K'R-KR)$ if $j'=j=2$.

Example. In Fig. 3 we plot the confined LO and TO mode spectra at $q=0$ for the particular case of a GaAs quantum wire, and modes confined to its interior. The velocity parameters c_{1L} and c_{1T} are both taken equal to 2900 ms^{-1}.[5] A wire radius $R=100$ Å is assumed. Figure 3 demonstrates that the confined frequency spectrum consists of multiplets of levels with $|m|=1,2,3,\ldots$, each multiplet corresponding to a certain value of K. Sublevels with $m=0$ behave extraordinarily. While they are located within the same K multiplet for TO_p modes, they belong to the $(K-1)$ multiplet for the LO and TO_s

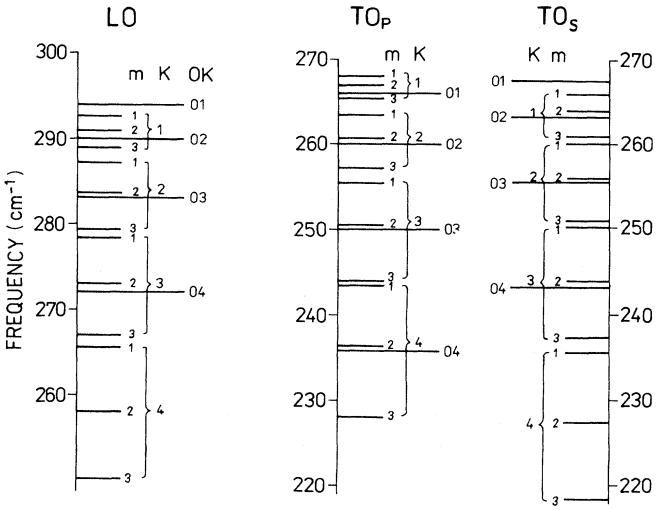

FIG. 3. Eigenfrequencies of confined optical-phonon modes at $q=0$ for a GaAs quantum wire of radius $R=100$ Å.

modes. The reason for the particular behavior of $m=0$ modes is that they are the only ones which may have nonvanishing angular averages of polarization charge densities. Sublevels within a given multiplet, i.e., with the same radial quantum number K but different axial quantum numbers m, are spaced by several cm^{-1}, corresponding to about 0.5 meV, while equivalent sublevels of different multiplets, i.e., with the same m but different K, have spacings several times larger. This means that the effect of radial confinement exceeds that of axial multiplicity by about half an order of magnitude. Typically, levels with equal m and with K differing by 1 have spacings around 10 cm^{-1}, corresponding to about 2 meV. Such small frequency distances are obtained in spite of the assumed small wire radius of 100 Å. If radii of several 1000 Å are taken, the frequency quantization turns out to be negligibly small.

V. INTERFACE MODES

According to Sec. II, the displacement fields $\mathbf{u}_{Imq}(\mathbf{x})$ of interface modes are characterized, first, by the vanishing of bulk sources and vortices:

$$\nabla\cdot\mathbf{u}_{Imq}(\mathbf{x})=0, \quad r\neq R \tag{48}$$

$$\nabla\times\mathbf{u}_{Imq}(\mathbf{x})=0, \quad r\neq R\ , \tag{49}$$

and, second, by the occurrence of discontinuities on the wire boundary $r=R$. By using these properties, the eigenvalue equation for IF modes becomes

$$[\omega_T^2(\mathbf{x})-\omega^2]\mathbf{u}_{Imq}(\mathbf{x})-\frac{e^*(r)}{M(r)}\hat{\mathbf{E}}_{mq}([\mathbf{u}_{Imq}(\mathbf{x})])=0\ , \quad r\neq R\ . \tag{50}$$

Here, $\hat{\mathbf{E}}_{mq}([\mathbf{u}_{Imq}(\mathbf{x})])$ means the electric field connected with an IF mode displacement field $\mathbf{u}_{Imq}(\mathbf{x})$. It represents a linear functional of $\mathbf{u}_{Imq}(\mathbf{x})$, which may be determined as follows.

In a first step we specify $\mathbf{u}_{Imq}(\mathbf{x})$. Owing to its general form (10) and due to the vanishing of bulk vortices, $\mathbf{u}_{Imq}$ may be expressed by a scalar potential

$$\psi_{Imq}(r)\exp[i(m\varphi+qz)]$$

as

$$\mathbf{u}_{Imq}(\mathbf{x})=\nabla[\psi_{Imq}(r)e^{i(m\varphi+qz)}], \quad r\neq R\ . \tag{51}$$

The vanishing of bulk sources of $\mathbf{u}_{Imq}(\mathbf{x},\omega)$ means that the Laplacian applied to

$$\psi_{Imq}(r)\exp[i(m\varphi+qz)]$$

vanishes. In cylindrical coordinates this condition reads

$$\left[\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\left[q^2+\frac{m^2}{r^2}\right]\right]\psi_{Imq}(r)=0, \quad r\neq R\ . \tag{52}$$

If taken to be valid in the whole infinite space including $r=R$, Eq. (52) defines the modified Bessel functions $I_m(qr)$ and $K_m(qr)$.[29,30] These functions have positive values and are nonzero for all r; $I_m(qr)$ remains finite at $r=0$ and diverges at $r=\infty$, while $K_m(qr)$ is infinite at $r=0$ and approaches zero at $r=\infty$. In our case, Eq. (52) holds only for $r<R$ and $r>R$. At $r=R$, $\psi_{Imq}(r)$ may have discontinuities. The normalization of the displacement fields means that $\psi_{Imq}(r)$ has to remain finite for all values of r, in particular, at $r=0$ and $r=\infty$. Two solutions of Eq. (52) exist with such properties. They read

$$b_{jmq}(\mathbf{x})=\Lambda_j(r)Z_{jm}(qr)e^{i(mq+qz)}, \quad j=1,2 \tag{53}$$

with

$$Z_{1m}(qr)=I_m(qr), \quad Z_{2m}(qr)=K_m(qr)\ . \tag{54}$$

The normalized vector fields $\mathbf{b}_{jmq}(\mathbf{x})$ attributed to $b_{jmq}(\mathbf{x})$ by means of Eq. (51) are

$$\mathbf{b}_{jmq}(\mathbf{x})=C_j\Lambda_j(r)\nabla[Z_{jm}(qr)^{i(m\varphi+qz)}], \quad j=1,2 \tag{55}$$

with normalization factors

$$C_1=\left[\frac{R}{2\Omega|q|}\frac{1}{I_m(qR)I'_m(qR)}\right]^{1/2}, \tag{56}$$

$$C_2=\left[\frac{R}{2\Omega|q|}\frac{-1}{K_m(qR)K'_m(qR)}\right]^{1/2}. \tag{57}$$

Note that $K'_m(qR)$ is negative for all q. The $\mathbf{b}_{jmq}(\mathbf{x})$, $j=1,2$, may be considered to form a set of orthonormalized basis functions within the space of vector fields having no bulk sources and vortices but sheet sources and vortices on the wire interface at $r=R$. Thus any IF mode displacement field $\mathbf{u}_{Imq}$ may be written as

$$\mathbf{u}_{Imq}(\mathbf{x})=\sum_j U_{Ijmq}\mathbf{b}_{jmq}(\mathbf{x})\ , \tag{58}$$

with U_{Ijmq} as arbitrary complex Fourier coefficients.

In a second step we calculate the electric field $\hat{\mathbf{E}}_{mq}([\mathbf{u}_{Imq}(\mathbf{x})])$ connected with an IF mode displacement field $\mathbf{u}_{Imq}(\mathbf{x})$. Since it represents a linear functional $\hat{\mathbf{E}}[\mathbf{u}_{Imq}(\mathbf{x})]$ of $\mathbf{u}_{Imq}(\mathbf{x})$, one has

$$\hat{\mathbf{E}}[\mathbf{u}_{Imq}(\mathbf{x})]=\sum_j U_{Ijmq}\hat{\mathbf{E}}[\mathbf{b}_{jmq}(\mathbf{x})]\ , \tag{59}$$

where $\hat{\mathbf{E}}[\mathbf{b}_{jmq}(\mathbf{x})]$ means the electric field due to the particular displacement field $\mathbf{b}_{jmq}(\mathbf{x})$. The bulk sources of $\hat{\mathbf{E}}[\mathbf{b}_{jmq}(\mathbf{x})]$ vanish since

$$\hat{\mathbf{E}}[\mathbf{b}_{jmq}(\mathbf{x})]=-4\pi e_j^* N_j \nabla\cdot\mathbf{b}_{jmq}(\mathbf{x})$$

holds, which gives zero because of Eqs. (51) and (52). The vortices of $\hat{\mathbf{E}}[\mathbf{b}_{jmq}(\mathbf{x})]$ are always zero owing to Maxwell's equation (3). Thus, $\hat{\mathbf{E}}[\mathbf{b}_{jmq}(\mathbf{x})]$ represents a vector field of IF-mode type by itself. As such, it may be linearly composed of IF-mode basis vectors $\mathbf{b}_{1mq}$ and $\mathbf{b}_{2mq}$. One has

$$\hat{\mathbf{E}}[\mathbf{b}_{jmq}(\mathbf{x})]=\sum_j E_{jj'mq}\mathbf{b}_{j'mq}(\mathbf{x})\ , \tag{60}$$

with $E_{jj'mq}$ as the Fourier components of $\hat{\mathbf{E}}[\mathbf{b}_{jmq}(\mathbf{x})]$. The latter are determined by the sheet sources of $\hat{\mathbf{E}}[\mathbf{b}_{jmq}(\mathbf{x})]$,

$$\nabla\cdot\{\varepsilon_\infty(\mathbf{x})\hat{\mathbf{E}}[\mathbf{b}_{jmq}(\mathbf{x})]\}=-4\pi e_j^* N_j C_j q Z_{jm}(qR)\delta(r-R)\ , \tag{61}$$

and by the vanishing of its sheet and bulk vortices, i.e.,

$$\nabla\times\hat{\mathbf{E}}[\mathbf{b}_{jmq}(\mathbf{x})]=0\ . \tag{62}$$

The two conditions (61) and (62) result in the following system of equations for $E_{jj'mq}$:

$$\begin{bmatrix}\epsilon_{1\infty}C_1 Z'_{1m}(qR) & -\epsilon_{2\infty}C_2 Z'_{2m}(qR)\\ C_1 Z_{1m}(qR) & -C_2 Z_{2m}(qR)\end{bmatrix}\begin{bmatrix}E_{j1mq}\\ E_{j2mq}\end{bmatrix}=(-1)^j 4\pi e_j^* N_j C_j\begin{bmatrix}Z'_{jm}(qR)\\ 0\end{bmatrix}\ . \tag{63}$$

By solving it, one arrives at

$$E_{jj'mq}=-\frac{4\pi e_j^* N_j}{\sqrt{\epsilon_{1\infty}\epsilon_{2\infty}}}M_{jj'}(m,q)\ , \tag{64}$$

with

$$\hat{M}(m,q)=\frac{1}{1+\alpha\eta_m(q)}\begin{bmatrix}1 & \sqrt{\alpha\eta_m(qR)}\\ \sqrt{\alpha\eta_m(qR)} & \alpha\eta_m(qR)\end{bmatrix}\ , \tag{65}$$

$$\eta_m(qR)=-\frac{I'_m(qR)K_m(qR)}{I_m(qR)K'_m(qR)},\quad \alpha=\frac{\epsilon_{2\infty}}{\epsilon_{1\infty}}\ . \tag{66}$$

Finally, the electric $\hat{\mathbf{E}}[\mathbf{u}_{Imq}(\mathbf{x})]$ of an IF-mode displacement field $\mathbf{u}_{Imq}(\mathbf{x})$ becomes

$$\hat{\mathbf{E}}[\mathbf{u}_{Imq}(\mathbf{x})]=\sum_{jj'}\frac{4\pi e_j^* N_j}{\sqrt{\epsilon_{1\infty}\epsilon_{2\infty}}}M_{jj'}U_{Ijmq}\mathbf{b}_{j'mq}(\mathbf{x})\ . \tag{67}$$

Since the matrix $M_{jj'}$ is symmetric, the operator $\hat{\mathbf{E}}$ turns out to be Hermitian on the subspace of IF modes, as it should be.

Expression (67) for $\hat{E}_{mq}([\mathbf{u}_{Imq}])$ will be used in order to specify the eigenvalue equation (50). As is commonly done, mass renormalized displacement components $(I|U_{mq}|j)$ are introduced instead of U_{Ijmq}. These are defined as

$$(I|U_{mq}|j)=\left[\frac{\rho_j}{M}\right]^{1/2}U_{Ijmq}\ , \tag{68}$$

where $\rho_j=N_j M_j$ means the reduced mass density of material j, and M abbreviates $\sqrt{M_1 M_2}$. The eigenvalue equation becomes

$$[\omega_{jT}^2-\omega^2](I|U_{mq}|j)+\sum_{j'}\omega_{jp}\omega_{j'p}M_{jj'}(I|U_{mq}|j')=0\ . \tag{69}$$

In matrix form it reads

$$\begin{bmatrix}\omega_{1T}^2+\omega_{1p}^2\dfrac{1}{1+\alpha\eta_m}-\omega^2 & \omega_{1p}\omega_{2p}\dfrac{\sqrt{\alpha\eta_m}}{1+\alpha\eta_m}\\ \omega_{1p}\omega_{2p}\dfrac{\sqrt{\alpha\eta_m}}{1+\alpha\eta_m} & \omega_{2T}^2+\omega_{2p}^2\dfrac{\alpha\eta_m}{1+\alpha\eta_m}-\omega^2\end{bmatrix}\times\begin{bmatrix}(I|U_{mq}|1)\\ (I|U_{mq}|2)\end{bmatrix}=\begin{bmatrix}0\\ 0\end{bmatrix}\ . \tag{70}$$

The two eigenvalues ω_{1mq}^2 and ω_{2mq}^2 of Eq. (69) for given m,q are

$$\omega_{Imq}^2=\frac{1}{2(1+\alpha\eta_m)}([\omega_{1L}^2+\omega_{2T}^2+\alpha\eta_m(\omega_{2L}^2+\omega_{1T}^2)]\pm\{[(\omega_{1L}^2-\omega_{2T}^2)+\alpha\eta_m(\omega_{2L}^2-\omega_{1T}^2)]^2+4\alpha\eta_m(\omega_{2L}^2-\omega_{1L}^2)(\omega_{2T}^2-\omega_{1T}^2)\}^{1/2})\ . \tag{71}$$

The lower $(-)$ sign corresponds to $I=1$, and the upper $(+)$ sign to $I=2$. The components $(I|U_{mq}|j)$ of displacement eigenfields are easily obtained from (70) and (71). By using them, the eigenfields $\mathbf{u}_{Imq}$ themselves become

$$\mathbf{u}_{Imq}(\mathbf{x})=\sum_j\left[\frac{M}{\rho_j}\right]^{1/2}(I|U_{mq}|j)\mathbf{b}_{jmq}(\mathbf{x})\ . \tag{72}$$

The Hermiticity of the dynamical operator in Eq. (69)

causes the 2×2 matrix $(I|U_{mq}|j)$ to be unitary, with the exception of a certain factor which becomes 1 for normalized displacement eigenfields. Thus one has

$$\sum_j (I|U_{mq}|j)(I'|U_{mq}|j)=\delta_{II'} , \tag{73}$$

$$\sum_I (I|U_{mq}|j)(I|U_{mq}|j')=\delta_{jj'} . \tag{74}$$

Equation (73) means orthonormalization of eigenfields in the sense

$$\left[\mathbf{u}_{Imq}\left|\frac{\rho(\mathbf{x})}{M}\right|\mathbf{u}_{I'mq}\right]=\delta_{II'} , \tag{75}$$

and Eq. (74) means completeness in the sense

$$\sum_I \left[\frac{\rho(\mathbf{x})}{M}\right]^{1/2}\left[\frac{\rho(\mathbf{x}')}{M}\right]^{1/2}\mathbf{u}_{Imq}(\mathbf{x})\mathbf{u}_{Imq}(\mathbf{x}') = \sum_j \mathbf{b}_{jmq}(\mathbf{x})\mathbf{b}_{jmq}(\mathbf{x}') . \tag{76}$$

IF-mode eigenfields are orthogonal to the eigenfields of any type $b=L,T_s,T_p$ of confined bulk modes. One has

$$(\mathbf{u}_{Imq}|\mathbf{u}_{jbKm'q'})=0, \quad b=L,T_s,T_p . \tag{77}$$

Dispersion relation from electrostatics

The dispersion relation (71) of IF-mode eigenfrequencies may also be obtained in a somewhat different way by using electrostatic equations only and by putting mechanics into the dielectric functions $\epsilon_j(\omega)$ of the two materials $j=1,2$. For $\epsilon_j(\omega)$, one has

$$\epsilon_j(\omega)=\epsilon_{j\infty}\left[1+\frac{\omega_{jp}^2}{\omega_{jT}^2-\omega^2}\right] . \tag{78}$$

The radial part of the scalar electric potential $\varphi_{Imq}(r)$ of an IF mode obeys the equation

$$\left[\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\left[q^2+\frac{m^2}{r^2}\right]\right]\varphi_{jmq}=0, \quad r\neq R . \tag{79}$$

Its finite solution reads

$$\varphi_{Imq}(r)=c_1\Lambda_1(r)I_m(qr)+c_2\Lambda_2(r)K_m(qr) , \tag{80}$$

with c_1,c_2 as unknown coefficients. The latter follow from continuity conditions at the wire interface; the parallel component of $\mathbf{E}_{Imq}$ and the normal component of $\mathbf{D}_{Imq}$ have to be continuous there. This yields

$$\begin{aligned} &I_m(qR)c_1-K_m(qR)c_2=0 , \\ &\epsilon_1(\omega)I_m'(qR)c_1-\epsilon_2(\omega)K_m'(qR)c_2=0 . \end{aligned} \tag{81}$$

The corresponding secular equation reads

$$\epsilon_1(\omega)+\eta_m(q)\epsilon_2(\omega)=0 . \tag{82}$$

By using expression (78) for $\epsilon_j(\omega)$, one may easily demonstrate that the eigenvalues ω_{Imq}^2 which follow from Eq. (82) are the same as those obtained previously from Eq. (70). Thus Eq. (82) represents an implicit form of the more explicit dispersion relation (71). Originally, this relation has been derived by Ruppin and Englman in Ref. 31.

Discussion of eigenmodes

First we consider the limit $qR\to\infty$. It holds that

$$\lim_{qR\to\infty}\eta_m(qR)=1 . \tag{83}$$

The dispersion relation (82) becomes

$$\epsilon_1(\omega)+\epsilon_2(\omega)=0 . \tag{84}$$

It is independent of m, and coincides with that of a single heterostructure possessing a plane interface. This is plausible since $qR\to\infty$ means that IF modes do not feel the curvature of the wire surface. The total number of different IF modes amounts to 2 in the limit $qR\to\infty$. For $qR\to0$, on the other hand, one gets

$$\lim_{qR\to0}\eta_m(qR)=\begin{cases}\infty & \text{for } m=0\\ 1 & \text{for } m\neq0 .\end{cases} \tag{85}$$

The singularity for $m=0$ modes is due to the fact that, in this case, the wire surface carries a nonvanishing net charge. For $m\neq0$ the charge vanishes. The two eigenfrequencies ω_{I00} for $m=0$ become $\omega_{100}=\omega_{1T}$ and $\omega_{200}=\omega_{2L}$, as long as $\omega_{2L}>\omega_{1T}$. The first of these modes is confined to material 1, and the second to material 2. If $\omega_{2L}<\omega_{1T}$, the meaning of the two modes is reversed. For $m\neq0$, the dispersion relations, and thus the eigenfrequencies, are the same in the two limiting cases $qR\to0$ and $qR\to\infty$. This represents a particular property of a cylindrical heterostructure. It becomes understandable if one realizes that $q\to0$ means independence of eigenfrequencies of the wire radius R. This includes large R, i.e., wires having an almost plane surface. Thus it is not surprising that, with the except of $m=0$, eigenfrequencies of plane heterostructures apply also to cylindrical heterostructures in the limit $q\to0$. Regarding all values of m, the total number of different mode frequencies amounts to 4 at $q=0$. For finite q, the dispersions of IF-mode eigenfrequencies and vectors follow from the q dependence of $\eta_m(qR)$. This function is plotted in Fig. 4 for the four lowest values of m.

Another case which needs particular consideration is that of a freestanding wire, i.e., a wire embedded in vacuum. In this case the IF-mode branch with $I=1$ becomes the surface mode branch $I=S$, and that with $I=2$ disappears. For $\omega_{1mq}\equiv\omega_{Smq}$, one gets from relation (71)

$$\omega_{Smq}^2=\omega_{1T}^2+\omega_{1p}^2\frac{\epsilon_{1\infty}}{\epsilon_{1\infty}+\eta_m(qR)} . \tag{86}$$

As a practical example, we consider a GaAs wire embedded either in AlAs or vacuum. In the AlAs case, GaAs-like and AlAs-like IF modes exist. The corresponding dispersion curves are plotted in Fig. 5. The eigenfrequencies of the surface mode branch belonging to the vacuum case are shown in Fig. 6. Since $\epsilon_{1\infty}\gg1$ for

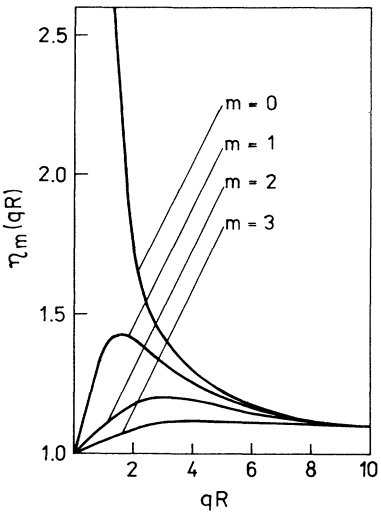

FIG. 4. Functions $\eta_m(q)$ determining the dispersion of IF modes.

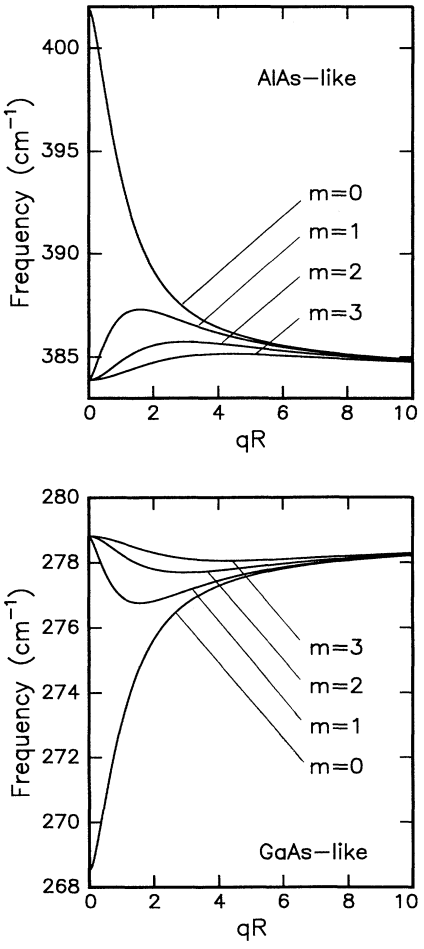

FIG. 5. Wave-vector dispersion of IF modes for a GaAs quantum wire embedded in AlAs.

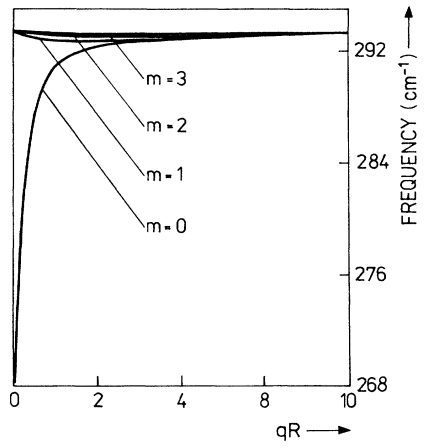

FIG. 6. Wave-vector dispersion of IF modes for a freestanding GaAs quantum wire.

GaAs, one gets $\omega_{Smq} \cong \omega_{1L}$ for $m \neq 0$, i.e., surface modes are almost degenerate with respect to m, and exhibit practically no q dispersion. For $m=0$, $\omega_{S00}=\omega_{1T}$ holds at $q=0$, and $\omega_{S0q} \cong \omega_{1L}$ for all other q except for very small ones.

VI. ELECTRON-PHONON INTERACTION

We consider the electron-phonon interaction of Fröhlich type. The interaction Hamiltonian differs for confined and interface modes.

Confined modes

We restrict ourselves to modes confined to the wire, i.e., to the material with $j=1$. No Fröhlich interaction exists for confined TO modes since their electric field $\mathbf{E}_{1TKmq}$ vanishes. For confined LO modes the dielectric displacement field $\mathbf{D}_{1LKmq}$ becomes zero. The electric field $\mathbf{E}_{1LKmq}$ is given by

$$\mathbf{E}_{1LKmq}(\mathbf{x}) = -4\pi e_1^* \epsilon_{1\infty}^{-1} N_1 \mathbf{u}_{1LKmq}(\mathbf{x}) . \tag{87}$$

By means of (22), (26), (28), and (29), the electrostatic potential $\varphi_{1LKmq}(\mathbf{x})$ due to $\mathbf{E}_{1LKmq}(\mathbf{x})$ may be expressed as

$$\varphi_{1LKmq}(\mathbf{x}) = 4\pi e_1^* \epsilon_{1\infty}^{-1} N_1 \left[\frac{1}{iq}\right] (\mathbf{e}_z \cdot \mathbf{u}_{1LKmq}) . \tag{88}$$

Any displacement field $\mathbf{u}_L$ of confined LO type represents a superposition of eigenfields $\mathbf{u}_{1LKmq}(\mathbf{x})$. One has

$$\mathbf{u}_L(\mathbf{x}) = \sum_{Kmq} U_{1LKmq} \mathbf{u}_{1LKmq}(\mathbf{x}) . \tag{89}$$

The normal coordinates U_{1LKmq} may be replaced by annihilation and creation operators B_{1LKmq} and B^+_{1LKmq}, defined by the relation

$$U_{1LKmq} = 2 \left[\frac{\hbar}{2\rho_1 \omega_{1LKmq}}\right]^{1/2} B_{1LKmq} . \tag{90}$$

The Fröhlich interaction Hamiltonian H_F equals to the

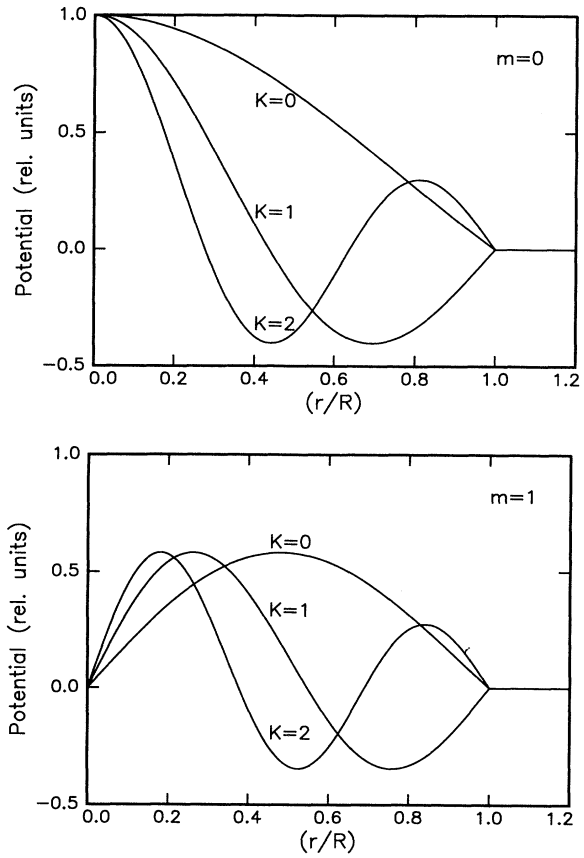

FIG. 7. Electrostatic potentials of LO modes confined to the wire. Various radial and axial quantum numbers K,m are shown.

real part of the total potential due to the displacement field $\mathbf{u}_L(\mathbf{x})$, multiplied by $-e$. It has the general form

$$H_F=\sum_{tmq}\{\varphi_{tmq}(r)\exp[i(m\varphi+qz)]B_{tmq} +\varphi_{tmq}(r)\exp[-i(m\varphi+qz)]B^{+}_{tmq}\}\ , \tag{91}$$

with $t=1LK$ and $\varphi_{tmq}(r)$ being the radial part of the potential multiplied by $-e$. One gets

$$\varphi_{1LKmq}(r)=\frac{e}{(q^2+K^2_{1Lm})^{1/2}} \times\left[\frac{2\pi\hbar\omega^2_{1p}}{\Omega\epsilon_{1\infty}\omega_{1LKmq}}\right]^{1/2}\theta(R-r) \times\frac{J_m(K_{1Lm}r)}{[-J_{m-1}(K_{1Lm}R)J_{m+1}(K_{1Lm}R)]^{1/2}}\ . \tag{92}$$

In Fig. 7, we plot $\varphi_{1LKmq}(r)$ for various radial and axial quantum numbers K,m.

Interface modes

The relation between the electric field $\hat{\mathbf{E}}[\mathbf{u}_{Imq}(\mathbf{x})]$ of an IF mode and its displacement eigenfield $\mathbf{u}_{Imq}(\mathbf{x})$ is less simple than for confined longitudinal modes. This is due to the nonvanishing vortices of $\mathbf{u}_{Imq}(\mathbf{x})$ which make the dielectric displacement field $\hat{\mathbf{D}}[\mathbf{u}_{Imq}(\mathbf{x})]$ differ from zero. We use a relation between $\hat{\mathbf{E}}[\mathbf{u}_{Imq}(\mathbf{x})]$ and $\mathbf{u}_{Imq}(\mathbf{x})$ which follows from the eigenvalue equation (50) observing relation (72). It reads

$$\hat{\mathbf{E}}[\mathbf{u}_{Imq}(\mathbf{x})]=\sum_j\left[\frac{4\pi M}{\epsilon_{j\infty}}\right]^{1/2}\frac{[\omega^2_{jT}-\omega^2_{Imq}]}{\omega_{jp}} \times(I|U_{mq}|j)\mathbf{b}_{jmq}(\mathbf{x})\ . \tag{93}$$

With the regard of expressions (55) for $\mathbf{b}_{jmq}(\mathbf{x})$, this field may be derived from an electrostatic potential $\varphi_{Imq}(\mathbf{x})$. If the normal coordinates $(I|U_{mq}|j)$ are replaced by annihilation and creation operators B_{Imq} and B^{*}_{Imq} defined by means of the relation

$$(I|U_{mq}|j)=2\left[\frac{\hbar}{2M\omega_{Imq}}\right]^{1/2}B_{Imq}\ , \tag{94}$$

one arrives at an interaction Hamiltonian H_F of the general form (91) with $t=I$ and the radial part of the potential $\varphi_{Imq}(\mathbf{x})$ given by the expression

$$\varphi_{Imq}(r)=\sum_j\left[\frac{e^2R\pi\hbar\omega_{Imq}}{|q|\Omega\epsilon_{j\infty}}\right]^{1/2}\frac{[\omega^2_{Imq}-\omega^2_{jT}]}{\omega_{Imq}\omega_{jp}}(I|U_{mq}|j) \times\left\{\delta_{j1}\theta(R-r)\frac{I_m(qr)}{[I_m(qR)I'_m(qR)]^{1/2}}+\delta_{j2}\theta(r-R)\frac{K_m(qr)}{[-K_m(qR)K'_m(qR)]^{1/2}}\right\}\ . \tag{95}$$

As shown by this expression, IF modes couple stronger the closer their frequencies approach those of longitudinal modes. The potentials $\varphi_{Imq}(r)$ of several IF modes of a freestanding GaAs wire are depicted in Fig. 8.

VII. CONCLUSIONS

In this paper we have derived the complete set of eigenfrequencies and displacement eigenfields of the optical-phonon modes of a circular quantum wire. The assumed circular shape is rather peculiar, but it makes an analytical treatment possible. This is important since the circular wire, owing to its full axial symmetry, may serve as reference case for arbitrary wires having necessarily lower symmetries. Moreover, certain general properties of optical-phonon modes of wires are independent of their particular shapes. Thus, the results of this paper are also useful for noncircular wires. The calculated

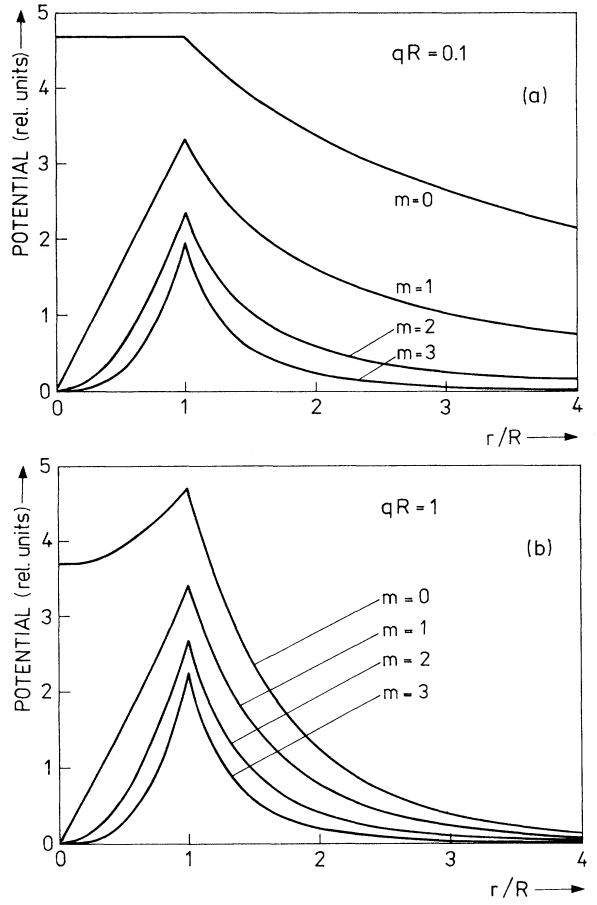

FIG. 8. Electrostatic potentials of the two IF mode branches of a freestanding GaAs wire for two different wave vectors q.

eigenfrequencies and eigenfunctions as well as Fröhlich interaction Hamiltonians allow one to study confinement and interface effects on optical-phonon modes for a variety of physical properties of quantum wires—among them Raman spectra, momentum scattering rates,[32] energy relaxation times, polaron effects, etc.

ACKNOWLEDGMENT

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APPENDIX

We consider an infinite, spatially homogeneous, and isotropic material. Its displacement eigenfields may be taken as plane waves:

$$(\mathbf{u}_{tQ}\mathbf{x})=\mathbf{e}_t e^{i\mathbf{Q}\cdot\mathbf{x}} \tag{A1}$$

of wave vector $\mathbf{Q}$ and polarization $\mathbf{e}_t$. The unit vectors $\mathbf{e}_t$ and $\mathbf{e}_L=\mathbf{Q}/Q$ for longitudinal modes ($t=L$) and $\mathbf{e}_{T_s}=\mathbf{e}_T$, $\mathbf{e}_{T_p}=[\mathbf{e}_L\times\mathbf{e}_T]$ for the two transverse modes ($t=T_s,T_p$), with $\mathbf{e}_T$ being an arbitrary unit vector perpendicular to $\mathbf{Q}$. The eigenfrequencies ω_{tQ} are degenerate for different directions of $\mathbf{Q}$. We use this degeneracy in order to construct eigenmodes of cylindrical symmetry with respect to an arbitrarity chosen z axis. The wave vector $\mathbf{Q}$ is decomposed into a component $\mathbf{K}$ perpendicular to $\mathbf{e}_z$ and a component q parallel to $\mathbf{e}_z$. By adopting the geometry of Fig. 2, one gets

$$\mathbf{Q}=K(\mathbf{e}_x\cos\varphi'+\mathbf{e}_y\sin\varphi')+q\mathbf{e}_z\ , \tag{A2}$$

where φ' means the polar angle of $\mathbf{Q}$. The polarization vectors $\mathbf{e}_L,\mathbf{e}_{T_s},\mathbf{e}_{T_p}$ become

$$\mathbf{e}_L=\frac{K}{Q}(\mathbf{e}_x\cos\varphi'+\mathbf{e}_y\sin\varphi')+\frac{q}{Q}\mathbf{e}_z\ , \tag{A3}$$

$$\mathbf{e}_{T_s}=-\mathbf{e}_x\sin\varphi'+\mathbf{e}_y\cos\varphi'\ , \tag{A4}$$

$$\mathbf{e}_{T_p}=\frac{q}{Q}(\mathbf{e}_x\cos\varphi'+\mathbf{e}_y\sin\varphi')-\frac{K}{Q}\mathbf{e}_z\ . \tag{A5}$$

If plane waves of the same polarization branch but different polar angles φ' are linearly combined with certain coefficients, one obtains again an eigenmode. We use coefficients $(1/2\pi)\exp(im\varphi')$, which depend on an integer m. The corresponding linear combinations are denoted by $\mathbf{g}_{tKmq}(\mathbf{x})$. They read

$$\mathbf{g}_{tKmq}(\mathbf{x})=\frac{1}{2\pi}\int_0^{2\pi}d\varphi' e^{im\varphi'}\mathbf{e}_t(\varphi')e^{i\mathbf{Q}\cdot\mathbf{x}}\ . \tag{A6}$$

We consider the components of $\mathbf{g}_{tKmq}(\mathbf{x})$ with respect to the cylindrical basis set $\mathbf{e}_r,\mathbf{e}_\varphi,\mathbf{e}_z$ at position $\mathbf{x}$. One obtains

$$\mathbf{g}_{tKmq}(\mathbf{x})=e^{i(m\varphi+qz)}\mathbf{w}_{tKmq}(r)\ , \tag{A7}$$

with the radial parts

$$\mathbf{w}_{LKmq}(r)=\frac{1}{2\pi}\int_0^{2\pi}d\varphi\left[\frac{K}{Q}\cos\varphi\cdot\mathbf{e}_r+\frac{K}{Q}\sin\varphi\cdot\mathbf{e}_\varphi+\frac{q}{Q}\mathbf{e}_z\right]\times e^{i(Kr\cos\varphi+m\varphi)}\ , \tag{A8}$$

$$\mathbf{w}_{T_sKmq}(r)=\frac{1}{2\pi}\int_0^{2\pi}d\varphi[-\sin\varphi\cdot\mathbf{e}_r+\cos\varphi\cdot\mathbf{e}_y]\times e^{i(Kr\cos\varphi+m\varphi)}\ , \tag{A9}$$

$$\mathbf{w}_{T_pKmq}(r)=\frac{1}{2\pi}\int_0^{2\pi}d\varphi\left[\frac{K}{Q}\cos\varphi\cdot\mathbf{e}_r+\frac{q}{Q}\sin\varphi\cdot\mathbf{e}_\varphi-\frac{K}{Q}\mathbf{e}_z\right]\times e^{i(Kr\cos\varphi+m\varphi)}\ . \tag{A10}$$

By using the relation

$$\frac{1}{2\pi}\int_0^{2\pi}d\varphi\, e^{i(Kr\cos\varphi+m\varphi)}=i^m J_m(Kr)\ , \tag{A11}$$

all φ integrals in (A8), (A9), and (A10) may be expressed by Bessel functions $J_m(Kr)$ of first kind and their deriva-

tives $J'_m(Kr)$.

Displacement fields calculated in this way are valid for an infinite homogeneous medium. In order to apply them to the interior of a wire, boundary conditions have to be set on the interface. For LO modes, i.e., modes without vortices, the parallel components of displacements fields have to be continuous, and for TO modes, i.e., modes without sources, continuity must hold for the normal components. These conditions are expressed by relation (30a) for LO modes and relations (39a) and (39b) for TO modes. Taking the boundary conditions into account, and omitting irrelevant phase factors and normalization constants, the displacement fields (A8), (A9), and (A10) turn out to be the same as those given by the expressions (29), (37), and (38), i.e., those obtained previously by means of the generalized Born-Huang equation.

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