Electron–LO-phonon interaction in semiconductor double heterostructures

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The electron–LO-phonon interaction Hamiltonian is deduced in a systematic way from a model of dispersive polar-optical vibrations for a semiconductor double heterostructure. LO phonons are introduced along the lines of the Born-Huang approach valid in the long-wavelength limit, while phonon confinement effects are included in a model which can be imagined as a jellium slab disposed between two rigid walls. The obtained Hamiltonian includes screening along the lines of the static three-dimensional (3D) Thomas-Fermi approximation and contains the 3D Frohlich Hamiltonian as a limiting case. The case of a single heterostructure is also contained as another limit. We compare our results with earlier works on the subject. Estimations of the polaronic energy shift and mass are reported.

I. INTRODUCTION

There is a growing interest in the investigation of semiconductor heterostructures like inversion layers, superlattices, multiple-quantum-well structures, and the like. In such systems electronic confined states are responsible for many new physical properties and effects with practical importance in the fabrication of new devices in micro- and optoelectronics.[1,2] Different physical quantities have been calculated for the above-mentioned structures,[2–9] where the usual materials are the weakly ionic III-V compounds (and alloys), such as GaAs/$Al_xGa_{1-x}As$ heterostructures. In these materials the electron–LO-phonon interaction plays an important role, especially for the description of transport and optical properties at high enough temperatures. In the study of free-carrier absorption of light,[6,9,10] scattering rates,[11] polaronic effects,[12,13] etc., the usual bulk Frohlich Hamiltonian for the electron–LO-phonon coupling has been utilized after invoking the good matching of the material elastic properties at the interfaces (and also considering almost equal dielectric properties).

However, presently it has been recognized that such an assumption could be certainly misleading. For instance, electron self-energies due to the electron–LO-phonon interaction are divergent if calculated by means of the bulk Frohlich Hamiltonian applied to a quasi-two-dimensional (Q2D) electron gas.[11] Although such divergences can be avoided by an appropriate consideration of screening,[11] they could also be surmounted if a more realistic model for LO phonons is utilized.

The effects of interface polar-optical phonons were considered in the investigation of layered heterostructures,[14,15] while experiments on magnetoabsorption and cyclotronic resonance in InSb inversion layers,[16] $Ga_xIn_{1-x}As$-InP superlattices,[17] and GaAs/$Al_xGa_{1-x}As$ heterostructures[18] confirmed that there are fundamental differences in the electron–LO-phonon interaction of semiconductor layered structures if compared with the strictly bulk case. Experiments on Raman scattering in superlattices and multiple-quantum-well structures[19,20] produced further concrete evidence about the important differences detected in the LO-phonon spectrum of the above-mentioned structures. Another effect which has been also considered is the contribution from image charges to the polarization field of the layered structure under the assumption of nonuniform dielectric constant.[21,22] Let us emphasize that for acoustic phonons the spectrum is not so deeply changed as in the case of polar-optical phonons. For polar-optical vibrations the possible modes have been numerically modeled for layered structures with the result that phonon modes are rather confined in each layer and the penetration of the vibrations into the adjacent layer is negligible.[23,24] All the above arguments support the now well-accepted fact of LO-phonon confinement in semiconductor layered structures and the need for a deduction of an electron–LO-phonon interaction Hamiltonian appropriate for such systems. Attempts in this direction can be already quoted. In Ref. 21 the Raman cross section in a double heterostructure (DHS) was investigated and, from an analysis of the inverse-dielectric-function poles, the electron–LO-phonon interaction Hamiltonian is obtained for a layered system using the potential created by the polarization field; in Ref. 15 the electron–LO-phonon Hamiltonian is induced from an analysis of the electron-energy-loss problem and, more recently, the superlattice case was considered under the assumption of a uniform dielectric constant and an *a priori* suggested polarization field that includes the LO-phonon confinement.[25]

The fundamental aim of the present work is to investigate electron–LO-phonon interaction in a DHS on the basis of a continuum (hydrodynamic) model for the long-wavelength polar-optical vibrations assuming they are dispersive and completely confined to the layer. We also assume uniform dielectric properties throughout the whole structure.

The assumed model for long-wavelength optical vibrations was suggested in Ref. 26 and resembles the Born-

Huang model but includes dispersion. In Sec. II we show how the equations of Ref. 26 for LO waves, entailing conditions of complete confinement in the DHS, can be solved; after that, the corresponding polarization field is derived and quantized. In Sec. III the electron–LO-phonon interaction Hamiltonian is deduced for a DHS using the already obtained polarization field; screening is included in the deduction from the very beginning on the basis of a three-dimensional (3D) static Thomas-Fermi approximation; the limiting cases of the bulk semiconductor and the single heterostructure are discussed. A completely second-quantized version of the Hamiltonian (including the confined electron system) is also obtained. In Sec. IV the particular case of completely confined electrons is briefly discussed and the obtained results are applied to the calculation of the polaronic energy shift and mass. Section V is devoted to the general conclusions.

II. POLARIZATION FIELD

We are only concerned with long-wavelength LO phonons and, therefore, a continuum approach along the lines of Born and Huang[27] for the classical vibrational field is appropriate, which, afterwards, must be properly quantized. As was remarked in Sec. I, a relatively simple hydrodynamic model was suggested recently[26] for polar-optical phonons in a DHS. In the framework of this model the dynamical equations for the lattice are written in the following form:

$$\ddot{\mathbf{u}}=-\omega_T^2\mathbf{u}+\left[\frac{1}{4\pi}(\epsilon_0-\epsilon_\infty)\right]^{1/2}\omega_T E - v_a^2\nabla(\nabla\cdot\mathbf{u})-v_b^2\nabla^2\mathbf{u}\ , \tag{1}$$

$$\mathbf{P}=\left[\frac{1}{4\pi}(\epsilon_0-\epsilon_\infty)\right]^{1/2}\omega_T\mathbf{u}+\frac{\epsilon_\infty-1}{4\pi}\mathbf{E}\ , \tag{2}$$

where $\mathbf{u}(\mathbf{r},t)$ is the effective ionic displacement (the units are such that $\mathbf{u}=\sqrt{\rho}\mathbf{w}$, where ρ is the mass density and $\mathbf{w}$ the real displacement field with units of length), ϵ_0 and ϵ_∞ are static and high-frequency dielectric functions, ω_T is the limiting (bulk) transverse-optical frequency, $\mathbf{E}$ is the electric field, $\mathbf{P}$ is the polarization field associated with the vibrations, and $\mathbf{v}_a$, $\mathbf{v}_b$ are vector parameters with dimensions of velocity. Equations (1) and (2) are analogous to those of Born and Huang[27] for an isotropic continuum but include dispersion effects through the terms proportional to $\mathbf{v}_a$ and $\mathbf{v}_b$; as discussed in Ref. 26, this dispersive modification of the Born and Huang equations is especially appropriate to account for the boundary conditions at the interfaces of the DHS.

For a charge-free (and current-free) system Eqs. (1) and (2) are supplemented by the Maxwell equations:

$$\nabla\cdot\mathbf{D}=0,\quad \nabla\cdot\mathbf{H}=0\ ,\qquad \nabla\times\mathbf{H}=\frac{1}{c}\dot{\mathbf{D}},\quad \nabla\times\mathbf{E}=-\frac{1}{c}\dot{\mathbf{H}}\ , \tag{3}$$

where the medium is assumed to be nonmagnetic and $\mathbf{D}=\mathbf{E}+4\pi\mathbf{P}$. Assuming $\mathbf{u}(\mathbf{r},t)=\mathbf{u}(\mathbf{r})\,e^{-i\omega t}$, we obtain

$$\mathbf{E}=\left[\frac{4\pi}{\omega_T^2}(\epsilon_0-\epsilon_\infty)^{-1}\right]^{1/2}[\omega_T^2-\omega^2+v_a^2\nabla(\nabla\cdot)+v_b^2\nabla^2]\mathbf{u}\ , \tag{4}$$

$$\mathbf{P}=[4\pi\omega_T^2(\epsilon_0-\epsilon_\infty)]^{-1/2}\times\{(\epsilon_0-1)\omega_T^2-(\epsilon_\infty-1)\omega^2+(\epsilon_\infty-1)[v_a^2\nabla(\nabla\cdot)+v_b^2\nabla^2]\}\mathbf{u}\ , \tag{5}$$

and

$$\mathbf{D}=\left[\frac{4\pi}{\omega_T^2}(\epsilon_0-\epsilon_\infty)^{-1}\right]^{1/2}\times\{\epsilon_0\omega_T^2-\epsilon_\infty\omega^2+\epsilon_\infty[v_a^2\nabla(\nabla\cdot)+v_b^2\nabla^2]\}\mathbf{u}\ . \tag{6}$$

Equations (1)–(3) are satisfied by a displacement field decomposed in the form $\mathbf{u}=\mathbf{u}_T+\mathbf{u}_L$, where $\nabla\cdot\mathbf{u}_T=0$, $\nabla\times\mathbf{u}_T\neq0$, $\nabla\cdot\mathbf{u}_L\neq0$, and $\nabla\times\mathbf{u}_L=0$.

For $\mathbf{u}_T$ the equation $\nabla\cdot\mathbf{D}=0$ is satisfied with $\mathbf{D}\neq0$ and the corresponding (dispersive) polariton modes are obtained. However, we are only interested in the longitudinal displacements $\mathbf{u}_L$ where the equation $\nabla\cdot\mathbf{D}=0$ is satisfied automatically because $\mathbf{D}=0$. For $\mathbf{u}_L(\mathbf{r},\omega)$ the following equation is obtained:

$$\left[\nabla^2+\frac{\omega_{\mathrm{LO}}^2-\omega^2}{v^2}\right]\mathbf{u}_L(\mathbf{r},\omega)=0\ , \tag{7}$$

where $\omega_{\mathrm{LO}}^2=(\epsilon_0/\epsilon_\infty)\omega_T^2$ (the familiar Lyddane-Sachs-Teller relation) and $v^2=v_a^2+v_b^2$. In the bulk case Eq. (7) leads to a quadratic dispersion law:

$$\omega_q^2=\omega_{\mathrm{LO}}^2-v^2q^2\ . \tag{8}$$

For the longitudinal electric and polarization fields we obtain

$$\mathbf{E}_L=-\left[\frac{4\pi\omega_{\mathrm{LO}}^2}{\epsilon^*}\right]^{1/2}\mathbf{u}_L \tag{9}$$

and

$$\mathbf{P}_L=\left[\frac{\omega_{\mathrm{LO}}^2}{4\pi\epsilon^*}\right]^{1/2}\mathbf{u}_L\ , \tag{10}$$

where $1/\epsilon^*=1/\epsilon_\infty-1/\epsilon_0$ (and therefore $\mathbf{D}_L=0$). Let us now consider a DHS with interfaces at $Z=0$ and $Z=a$ (the Z axis is perpendicular to the interfaces). For $0<Z<a$ we have a given material (say, GaAs) and for $Z<0$ and $Z>a$ we have another material (say, $Al_xGa_{1-x}As$). In Ref. 26 boundary conditions of continuous $\rho^{-1/2}\dot{u}_Z$ and $v^2\rho^{1/2}\nabla\cdot\mathbf{u}$ at the interfaces are imposed along the lines of an hydrodynamic (or jellium) model; the first quantity is the Z component of the velocity field and the second quantity is the pressure. We will not discuss the more general solution of Ref. 7, but rather the one entailing complete confinement of the LO vibrations. This particular form of vibrations should provide an appropriate description for the observed highly confined LO phonons (see sec. I). Therefore, we solve Eq.

(7) under the following requirements:

$$u_Z(\mathbf{r},\omega)=0 \quad \text{for } Z=0 \text{ and } Z=a \tag{11}$$

(from now on subscript L is avoided and $\mathbf{u}$ will describe purely longitudinal vibrations). Conditions (11) involve a "jellium" slab disposed between rigid walls at $Z=0$ and $Z=a$ as a macroscopic model for completely confined LO vibrations, that is, a model excluding penetration of the polar-optical vibrations from a given layer into the adjacent ones. We must emphasize that this kind of model is in good agreement with experimental facts[19,20] and numerical simulations,[24] and also provides the possibility of working out analytical expressions for the displacement and polarization fields.

After substitution of $\mathbf{u}(\mathbf{r})=\xi(Z)e^{i\mathbf{q}_\perp\cdot\mathbf{r}_\perp}$ in (7) we obtain

$$\left[\frac{d^2}{dZ^2}+q_Z^2\right]\xi(Z)=0 , \tag{12}$$

where

$$q_Z^2=\frac{1}{v^2}(\omega_{\mathrm{LO}}^2-\omega^2)-q_\perp^2\geq 0$$

and

$$\xi_Z(0)=\xi_Z(a)=0 .$$

For $q_Z^2>0$ the solution of (12) is

$$\xi(Z)=A[(\mathbf{q}_\perp+q_Z\mathbf{e}_Z)e^{iq_ZZ}+(\mathbf{q}_\perp-q_Z\mathbf{e}_Z)e^{-iq_ZZ}] , \tag{13}$$

with

$$q_Z=\frac{n\pi}{a}$$

and

$$n=1,2,3,\ldots .$$

Let us note that (13) satisfies Eq. (12) with the given boundary conditions and, when substituted in the expression for $\mathbf{u}$, ensures the condition $\nabla\times\mathbf{u}=0$ for the longitudinal displacements. It is easy to include the case $q_Z=0$ just allowing n to be zero in (13). For $q_Z^2<0$ no solutions exist satisfying the given boundary conditions.

From (13) we obtain the general solution for

$$\mathbf{u}(\mathbf{r})=\sum_{\mathbf{q}_\perp}\sum_{n\geq 0}A_{\mathbf{q}_\perp,n}[(\mathbf{q}_\perp+q_Z\mathbf{e}_Z)e^{iq_ZZ}+(\mathbf{q}_\perp-q_Z\mathbf{e}_Z)e^{-iq_ZZ}]e^{i\mathbf{q}_\perp\cdot\mathbf{r}_\perp} , \tag{14}$$

where $q_Z=n\pi/a$ and $A_{\mathbf{q}_\perp,n}$ are constant parameters. Let us note that the sums over $\mathbf{q}_\perp$ and n cannot be infinite. We must require $\omega^2=\omega_{\mathrm{LO}}^2-v^2q^2>0$ (only if $v\to 0$ do we obtain infinite sums). We should agree to sum in the following way: n will be summed in the interval $0<n<N(q_\perp)$ where $N(q_\perp)$ is the higher integer less than $(\omega_{\mathrm{LO}}^2/v^2-q_\perp^2)^{1/2}$ for a fixed $q_\perp$; after that, $\mathbf{q}_\perp$ will be summed for all values inside the circle limited by $q_\perp^2=q_x^2+q_y^2=(\omega_{\mathrm{LO}}/v)^2$. Notice that the change $\mathbf{q}_\perp$ by $-\mathbf{q}_\perp$ does not alter the latter summation. Expression (14) can be transformed into

$$\mathbf{u}(\mathbf{r})=\sum_{\mathbf{q}}\sum_{n=-N(q_\perp)}^{N(q_\perp)}\mathbf{q}(A_{\mathbf{q}_\perp,|n|}e^{i\mathbf{q}\cdot\mathbf{r}}+A^*_{\mathbf{q}_\perp,|n|}e^{-i\mathbf{q}\cdot\mathbf{r}}) \tag{15}$$

with $\mathbf{q}=\mathbf{q}_\perp+q_Z\mathbf{e}_Z$ and $A^*_{\mathbf{q}_\perp,|n|}=-A_{-\mathbf{q}_\perp,|n|}$, the latter condition ensuring that $\mathbf{u}$ is a real quantity.

Obviously, Eqs. (15) and (14) are completely identical expressions, but (15) is more convenient in what follows. Substitution of (15) in (10) yields $\mathbf{P}(\mathbf{r},t)$, the polarization field, while the corresponding canonical conjugate momentum is given by[28]

$$\Pi(\mathbf{r},t)=\frac{4\pi\epsilon^*}{\omega_{\mathrm{LO}}^2}\frac{\partial\mathbf{P}(\mathbf{r},t)}{\partial t} . \tag{16}$$

The parameters $A_{\mathbf{q}_\perp,|n|}$ must be chosen appropriately in order that the corresponding quantized fields $\hat{\mathbf{P}}$ and $\hat{\Pi}$ can satisfy adequate commutation relations.[28]

We just report the final expression form $\hat{\mathbf{P}}(\mathbf{r})$:

$$\hat{\mathbf{P}}(\mathbf{r})=\sum_{\mathbf{q}_\perp}\sum_{n=-N(q_\perp)}^{N(q_\perp)}\left[\frac{\hbar\omega_{\mathrm{LO}}^2}{8\pi\epsilon^*\omega_q V}\right]^{1/2}\frac{\mathbf{q}}{|\mathbf{q}|}\times(e^{i\mathbf{q}\cdot\mathbf{r}}\hat{b}_{\mathbf{q}}+\text{c.c.}) , \tag{17}$$

where $\hat{b}_{\mathbf{q}}$, $\hat{b}^\dagger_{\mathbf{q}}$ are second-quantization Bose operators such that

$$\begin{aligned}&[\hat{b}_{\mathbf{q}},\hat{b}_{\mathbf{q}'}]=[\hat{b}^\dagger_{\mathbf{q}},\hat{b}^\dagger_{\mathbf{q}'}]=0 ,\\ &[\hat{b}_{\mathbf{q}},\hat{b}^\dagger_{\mathbf{q}'}]=\delta_{\mathbf{q},\mathbf{q}'} .\end{aligned} \tag{18}$$

Expression (17) is the fundamental result of this section which must be used to derive the electron–LO-phonon Hamiltonian for a DHS. The main difference with respect to the usual (bulk) polarization field is the discrete nature of $q_Z=n\pi/a$ and the fact that $\mathbf{P}(\mathbf{r})$ is defined just for the layer $0<Z<a$.

III. INTERACTION HAMILTONIAN

The interaction Hamiltonian can be deduced from[28]

$$\hat{H}_I(\mathbf{r})=\int\frac{e[-\nabla'\cdot\hat{\mathbf{P}}(\mathbf{r}')]}{|\mathbf{r}-\mathbf{r}'|}e^{-|\mathbf{r}-\mathbf{r}'|/\lambda}d^3r' , \tag{19}$$

where, for the sake of generality, we have included a screening length λ along the lines of the (bulk) Thomas-Fermi static approximation. Let us, however, remark that the obtained results are perfectly valid in the limit $\lambda\to\infty$.

Substitution of (17) in (19) yields, after straightforward integrations, the following Hamiltonian for the DHS:

$$\hat{H}_I^{\mathrm{DHS}} = \sum_{\mathbf{q}_\perp} \sum_{n=-N(q_\perp)}^{N(q_\perp)} [C_{\mathbf{q},\lambda} e^{i\mathbf{q}\cdot\mathbf{r}} \Phi_{\mathbf{q},\lambda}^{\mathrm{DHS}}(Z) \hat{b}_{\mathbf{q}} + \mathrm{c.c.}] , \quad (20)$$

where

$$C_{\mathbf{q},\lambda} = -ie \left[\frac{2\pi\hbar\omega_{\mathrm{LO}}^2}{\omega_q \epsilon^* V} \right]^{1/2} \frac{q}{q^2 + 1/\lambda^2} \quad (21)$$

is the usual (screened) coupling factor of the bulk theory (the unscreened coupling factor is defined by $C_{\mathbf{q}} = \lim_{\lambda\to\infty} C_{\mathbf{q},\lambda}$) and

$$\Phi_{\mathbf{q},\lambda}^{\mathrm{DHS}}(Z) = \begin{cases} \frac{1}{2} e^{(Q - iq_Z)Z} [1 - (-1)^n e^{-Qa}] & \text{for } Z < 0 , \\ 1 - \frac{1}{2} e^{-iq_Z Z} [e^{-QZ} + (-1)^n e^{Q(Z-a)}] & \text{for } 0 < Z < a , \\ \frac{1}{2} e^{-(Q + iq_Z)Z} [(-1)^n e^{Qa} - 1] & \text{for } Z > a , \end{cases} \quad (22)$$

where $Q^2 = q_\perp^2 + 1/\lambda^2$.

The structure of $\hat{H}_I^{\mathrm{DHS}}$ is very clear from the physical side. Due to LO-phonon confinement the Z component of the phonon wave vector $\mathbf{q}$ bears a discrete nature; the coupling factor $C_{\mathbf{q},\lambda}$ is the same as in the bulk (screened) Frohlich Hamiltonian, but now a certain modulation function $\Phi_{\mathbf{q},\lambda}^{\mathrm{DHS}}(Z)$ is present describing the effect of confinement; in fact we must notice that $\Phi_{\mathbf{q},\lambda}^{\mathrm{DHS}}(Z)$ is evanescent for $Z < 0$ or $Z > a$; for $0 < Z < a$, $\Phi_{\mathbf{q},\lambda}^{\mathrm{DHS}}(Z)$ has two terms: the first term (equal to unity) is just the bulk-like contribution, while the second term involves two contributions coming from the interfaces at $Z = 0$ and $Z = a$. The unscreened limit ($\lambda \to \infty$), is obtained without difficulties just taking $Q \to q_\perp$ in (22) and the corresponding expression for (21). A more realistic screening theory can be obtained from the unscreened $\hat{H}_I$ just dividing $C_{\mathbf{q}}$ by a proper dielectric function $\epsilon(\mathbf{q},\omega)$ (see, for instance, Ref. 1). Nevertheless, our screened formula for $\hat{H}_I$ provides a certain estimation of screening effects of qualitative importance and can be handled analytically.

One important feature of the obtained expressions [(20)–(22)] is that the three-dimensional (3D) (bulk) limiting case can be achieved if we firstly shift the coordinate origin by means of $Z = Z' + a/2$ and, afterwards, take the limit $a \to \infty$. Hence we obtain the well-known screened Fröhlich Hamiltonian (for dispersive LO phonons):

$$\hat{H}_I^{\mathrm{3D}}(\mathbf{r}) = \sum_{\mathbf{q}} (C_{\mathbf{q},\lambda} e^{i\mathbf{q}\cdot\mathbf{r}} \hat{b}_{\mathbf{q}} + \mathrm{c.c.}) . \quad (23)$$

Another important limiting case can be deduced from our expressions if we directly take $a \to \infty$ in (20)–(22). This is the case of the single heterostructure (SHS) where

$$\Phi_{\mathbf{q},\lambda}^{\mathrm{SHS}}(Z) = \begin{cases} \frac{1}{2} e^{(Q - iq_Z)Z}, & Z < 0 \\ 1 - \frac{1}{2} e^{-(Q + iq_Z)Z}, & Z > 0 . \end{cases} \quad (24)$$

Substitution of (24) in place of $\Phi_{\mathbf{q},\lambda}^{\mathrm{DHS}}$ in (20) provides the given Hamiltonian $\hat{H}_I^{\mathrm{SHS}}(\mathbf{r})$.

We should emphasize that our expressions [(20)–(24)] contain in a well-defined way the nondispersive approximation just taking $v \to 0$ and $\omega_{\mathbf{q}} \to \omega_{\mathrm{LO}}$. This approximation is justified for the long-wavelength LO phonons considering that v is small enough (in Ref. 26, v is estimated as $\sim 5 \times 10^5$ cm/s) and, therefore, $vq \ll \omega_{\mathrm{LO}}$. Let us note that the dispersive model for LO phonons used in this work is needed in order to account for the boundary conditions of a DHS, but once the expressions for $\hat{\mathbf{P}}(\mathbf{r})$ and $\hat{H}_I(\mathbf{r})$ are obtained we can safely take the nondispersive limit for which the calculations are evidently easier. In this case $N_{q_\perp} \to \infty$ and the involved summations are both infinite and well defined.

In the DHS case we can describe the confined electron system by means of the quantum field

$$\hat{\Psi}(\mathbf{r}) = \sum_{\mathbf{k}_{\perp},l} \frac{1}{\sqrt{S}} e^{i\mathbf{k}_\perp \cdot \mathbf{r}_\perp} \phi_l(Z) \hat{a}_{\mathbf{k}_{\perp},l} , \quad (25)$$

where S is the normalization area parallel to the interfaces, $\mathbf{k}_\perp \equiv (k_X, k_Y)$ is the electron wave vector for the motion in the (X, Y) plane, $\phi_l(Z)$ are the wave functions for the motion of the electrons in the confinement direction, and $\hat{a}_{\mathbf{k}_{\perp},l}$ is the annihilation operator of an electron in the state $\mathbf{k}_{\perp},l$. A completely second-quantized version of the electron–LO-phonon interaction Hamiltonian can be obtained from

$$\hat{H}_I^{\mathrm{DHS}} = \int \hat{\Psi}^\dagger(\mathbf{r}) \hat{H}_I^{\mathrm{DHS}}(\mathbf{r}) \hat{\Psi}(\mathbf{r}) d^3r . \quad (26)$$

By means of (20), (25), and (26) we obtain

$$\hat{H}_I^{\mathrm{DHS}} = \sum_{\mathbf{k}_{\perp},l} \sum_{\mathbf{k}'_{\perp},l'} \sum_{\mathbf{q}} [\Gamma_{ll'n}(\mathbf{q}_\perp, \mathbf{k}_\perp, \mathbf{k}'_\perp) \hat{b}_{\mathbf{q}} \hat{a}^\dagger_{\mathbf{k}_{\perp},l} \hat{a}_{\mathbf{k}'_{\perp},l'} + \mathrm{c.c.}] , \quad (27)$$

where

$$\Gamma_{ll'n}(\mathbf{q}_\perp, \mathbf{k}_\perp, \mathbf{k}'_\perp) = \delta_{\mathbf{k}_\perp, \mathbf{k}'_\perp + \mathbf{q}_\perp} \Gamma_{ll'n}(\mathbf{q}_\perp) \quad (28)$$

and

$$\Gamma_{ll'n}(\mathbf{q}_\perp) = C_{\mathbf{q},\lambda} \int \phi_l^*(Z) \phi_{l'}(Z') e^{iq_Z Z} \Phi_{\mathbf{q},\lambda}^{\mathrm{DHS}}(Z) dZ . \quad (29)$$

For the calculation of the form factor $\Gamma_{ll'n}(\mathbf{q}_\perp)$ the electron wave function $\phi_l(Z)$ must be specified. We should emphasize that no restrictions in the nature of $\phi_l(Z)$ are

assumed in our deductions. The Hamiltonian (27) involves more information than (20), as far as the electron quantities are explicitly included.

IV. FORM-FACTOR FOR COMPLETELY CONFINED ELECTRONS

An interesting application of the above-obtained expressions is the case when the electrons in a DHS are completely confined due to infinite potential barriers at $Z=0$ and $Z=a$. In this case,

$$\phi_l(Z)=\begin{cases}\left[\frac{2}{a}\right]^{1/2}\sin\left[\frac{\pi l}{a}Z\right] & \text{for } 0<Z<a\ ,\\ 0 & \text{for other values of } Z\ .\end{cases} \tag{30}$$

Substitution of (30) in (29) provides the corresponding form factor. After more or less straightforward mathematical manipulations, we have obtained the following result:

$$\Gamma_{ll'n}(\mathbf{q}_\perp)=J_{ll'n}+\frac{2\pi^2 Qall'C_{q,\lambda}[1+(-1)^{l+l'+n}]}{[Q^2a^2+\pi^2(l+l')^2]}\times\frac{[(-1)^n e^{-Qa}-1]}{[Q^2a^2+\pi^2(l-l')^2]}\ , \tag{31}$$

where

$$J_{ll'n}=\begin{cases}C_{q,\lambda} & \text{for } l=l' \text{ and } n=0\ ,\\ -\frac{1}{2}C_{q,\lambda} & \text{for } n=\pm(l+l')\ ,\\ \frac{1}{2}C_{q,\lambda} & \text{for } n=\pm(l-l') \text{ and } l-l'\ .\end{cases} \tag{32}$$

Expression (31) can be used to estimate the polaronic energy shift and effective mass for the case of a weak-coupling polaron and $T=0$ K. This can be deduced from perturbation theory up to the second order[28] by a well-known procedure. Avoiding details, we just report the obtained results:

$$\varepsilon_{\mathbf{k}_{\perp,l}}-\varepsilon^{(0)}_{\mathbf{k}_{\perp,l}}\simeq-\alpha_l\hbar\omega_{\mathrm{LO}}-\frac{\hbar^2k_\perp^2}{2m_l}\ , \tag{33}$$

where

$$\varepsilon^{(0)}_{\mathbf{k}_{\perp,l}}=\frac{\hbar^2k_\perp^2}{2m}+E_0l^2,\quad E_0=\frac{\pi^2\hbar^2}{2ma^2}\ , \tag{34}$$

$$m_l=m(1-\gamma_l)^{-1}\ . \tag{35}$$

Parameters α_l and γ_l determine the polaronic energy shift and effective mass, respectively (in the parabolic approximation), assuming the electron in the l subband and considering all intersubband and intrasubband transitions induced by the electron–LO-phonon interaction. We obtain that

$$\alpha_l=16\pi\alpha\left[\frac{\hbar\omega_{\mathrm{LO}}}{E_0}\right]^{1/2}\sum_{l'}F^{(1)}_{ll'} \tag{36}$$

and

$$\gamma_l=32\pi^3\alpha\left[\frac{\hbar\omega_{\mathrm{LO}}}{E_0}\right]^{3/2}\sum_{l'}F^{(3)}_{ll'}\ , \tag{37}$$

where $F^{(j)}_{ll'}$ $(j=1,3)$ are functions of $\hbar\omega_{\mathrm{LO}}$ which will not be reported explicitly in the present work and

$$\alpha=\frac{e^2m^{1/2}}{2^{1/2}\hbar^{3/2}\epsilon^*\omega_{\mathrm{LO}}^{1/2}} \tag{38}$$

is the Fröhlich constant. Let us note that the 3D theory predicts $\alpha_l\to\alpha$ and $\gamma_l\to\alpha/6$,[28] while the strictly 2D theory predicts $\alpha_1\to(\pi\alpha)/2$, $\gamma_1\to\pi\alpha/8$.[12,13] Our evaluation of α_l and γ_l for $l=1$ in a DHS of GaAs with $a=100$ Å and taking $\lambda\to\infty$ yields

$$\alpha_1\simeq1.6\alpha,\quad \gamma_1\simeq0.37\alpha\ ,$$

which are larger than the 3D case but lower than the 2D case. An investigation of the polaronic effects on the basis of the Hamiltonian deduced in the present paper deserves an independent work to be published in the near future.

V. CONCLUSIONS

The main contribution of the present work is the systematic deduction of an electron–LO-phonon interaction Hamiltonian for a semiconductor DHS incorporating the peculiarities of dispersive confined LO phonons. Our deduction is based upon a relatively simple model for long-wavelength phonons, considering a continuum (hydrodynamic) approach and assuming a phonon dispersion law quadratic with the wave vector [see Eq. (8)] where $q_Z=n\pi/a$ is discrete. This model for the LO phonons is in very good agreement with experimental results on Raman scattering in superlattices for a $GaAs/Al_xGa_{1-x}As$ heterostructure[19] [compare with expression (12) and Fig. 9 of Ref. 19]. As was emphasized in Sec. I, this model is also in good agreement with other experimental facts (for instance, experiments on the magnetophonon effect[29]) and with numerical simulations of the polar-optical vibrations,[24] where it was clearly determined that the penetration of optical vibrations from one layer to the adjacent ones is rather negligible.

The general structure of the Hamiltonian obtained in the present work resembles the Hamiltonian induced in Ref. 15 from electron-energy-loss expressions (where the author also considers the effects of a certain system of "modified" image charges, by means of which the possibility of different dielectric constants is included). However, some differences between our results and those of Ref. 15 can be easily noted, especially in the coefficients, and therefore the predicted intensities of the electron–LO-phonon interaction are not the same.

One important advantage of our results is that they contain the usual 3D Fröhlich Hamiltonian as a limiting case. Another advantage is that we worked out an explicit model for polar-optical vibrations, a model which is reasonable from intuitive physical grounds and in good agreement with experimental facts as has been stressed in the above discussions. Of course, the possibility of assuming more realistic conditions for the utilized model is

always present for this kind of deductions (for instance, we could assume different dielectric constants in the system or not completely confined LO phonons). However, one important aspect to be pointed out is that our results are relatively simple analytical expressions.

For the case of a superlattice the electron–LO-phonon interaction Hamiltonian was proposed in Ref. 25 assuming uniform dielectric constant throughout the structure. The author supports his deductions on an *a priori* suggested formula for the polarization field (which seems to be plausible for intuitive physical reasons). We think that our results, properly extended to the superlattice case, could be used to verify the Hamiltonian of Ref. 25.

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