A many-particle approach to the electron-phonon interaction in semiconductor nanostructures

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A new, many-particle approach to the interaction between electrons and polar optical phonons in semiconductor nanostructures, in which the statistical average over phonon states is exactly performed, is presented. The interaction is then reduced to an effective retarded electron-electron one. As an application, the polaron free energy is calculated from the first-order correction to the thermodynamical potential within the framework of a dispersive electroelastic continuum model for the long-wavelength polar optical oscillations in a GaAs/AlAs double heterostructure.

Keywords: Polaron free-energy; semiconductor heterostructures

Se presenta un nuevo formalismo para el estudio de la interacción entre los electrones y los fonones ópticos polares en heteroestructuras semiconductoras, en el cual se realiza de forma exacta la promediación sobre los estados del subsistema fonónico, de modo que la interacción electrón-fonón se reduce a una interacción retardada efectiva entre los electrones. Como aplicación del formalismo se calcula la energía libre del polarón en una heteroestructura doble del tipo GaAs/AlAs a partir de la corrección perturbativa de primer orden al potencial termodinámico en el marco de un modelo electroelástico continuo para las oscilaciones ópticas polares de longitud de onda larga.

Descriptores: Energía libre polarónica; heteroestructuras semiconductoras

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1. Introduction

The polar optical phonons in semiconductor layered structures have become a subject of much theoretical investigation and several phenomenological models for the long-wavelength polar optical oscillations in those systems have been put forward for heterostructures of different types of geometries. Within this framework, electron-phonon interaction Hamiltonians can be derived under general conditions [1–9].

The problem of averaging over phonon variables was presented for the first time by Feynman [10], who applied his variational path-integral method to study the polaron in bulk systems, and performed an exact reduction of the electron-phonon interaction to a retarded interaction between electrons. Posteriorly, different versions of that method were systematically used to calculate the polaron properties in the bulk case [11, 12].

An alternative procedure for the elimination of the phonon variables in the polaron problem—which is mathematically rigorous and is based on second quantization—was proposed by Bogolubov and Bogolubov [13]. In the present work, Bogolubov's method is extended to deal with the many-electron system interacting with polar optical phonons in semiconductor planar layered heterostructures, such as superlattices, multiple quantum wells, single and double heterostructures, etc. The consideration of planar interfaces is due mostly to simplicity. It will result obvious that our approach is valid for any type of structure, independently of its geometry, so that one could account for systems like quantum wires, quantum dots, etc. The differences will come from the specific form of the electronic states and the interaction Hamiltonian for each particular situation.

The evaluation of the polaron free energy is one of the direct results of the path-integral formalism in bulk systems (see, for instance, Refs. 12, 14 and 15). However, this quantity does not seem to have been so far widely calculated in low-dimensional heterostructures due to the explicit difficulties for the application of a Feynman-like procedure in systems bearing interfaces. An alternative way is the use of the perturbative method coming from a Green's function approach to the thermodynamical potential. In the case of semiconducting materials like the III-V and II-VI compounds, the magnitude of the electron-phonon coupling constants are small enough to allow for a perturbative treatment usually restricted -at most- to the second order corrections. Therefore, such a calculation process can be carried out as well in the case of semiconducting heterostructures made from those materials.

Here, we are going to use the many-particle Green's function-based formalism resulting from the extension of the Bogolubov's method to evaluate the polaron free energy as a function of the temperature in the case of a GaAs/AlAs quantum well. The paper is organized as follows. In Sec. 2 we start describing the Hamiltonian of the electron-phonon system and then discuss the reduction of the statistical operator after the averaging over phonon variables. Section 3 is devoted to the study of the one-electron Green's function and the subsequent derivation of the thermodynamical potential.

In Sec. 4, the approach is applied to the evaluation of the polaron free energy in the mentioned system, according to the so-called dispersive electroelastic continuum model (DECM) for the polar optical phonons [16]. Section 5 contains the conclusions of the work.

2. Reduced statistical operator of the electronic subsystem

The Hamiltonian for the electron-phonon system in the heterostructure is

$$\hat{H} = \hat{H}_{\rm e} + \hat{H}_{\rm ph} + \hat{H}_{\rm e-ph}. \tag{1}$$

$\hat{H}_{\rm e}$ is the Hamiltonian of the non-interacting electronic subsystem which consists of the electrons in a given energy band. The one-electron states are described within the envelope function approximation and obey certain effective mass differential equation. In a planar layered heterostructure, the appropriate quantum numbers which describe these states are the in-plane wavevector $\mathbf{k} = (k_x, k_y)$ and ζ, a quantum number associated to the motion of the electron along the growth direction (assumed to be "z"). If we introduce $\hat{a}_{\mathbf{k}\zeta}$ and $\hat{a}^{\dagger}_{\mathbf{k}\zeta}$: the annihilation operator and the creation operator, of an electron in the state $|\mathbf{k}, \zeta\rangle$, respectively, the Hamiltonian $\hat{H}_{\rm e}$ is written as

$$\hat{H}_{\rm e} = \sum_{\mathbf{k},\zeta} E_{\mathbf{k},\zeta} \hat{a}^{\dagger}_{\mathbf{k}\zeta} \hat{a}_{\mathbf{k}\zeta}. \tag{2}$$

The Hamiltonian $\hat{H}_{\rm ph}$ corresponds to the non-interacting phonon subsystem. Regardless the particular long-wavelength model to be considered for the study of the polar oscillations, the dispersion relations can be designated, in general, by $\omega_s(\mathbf{q})$, where the in-plane wavevector $\mathbf{q} = (q_x, q_y)$ and the index "s" particularizes the specific mode. The form of this Hamiltonian is

$$\hat{H}_{\rm ph} = \sum_{\mathbf{q},s} \hbar\omega_s(\mathbf{q}) \hat{b}^{\dagger}_{\mathbf{q}s} \hat{b}_{\mathbf{q}s}. \tag{3}$$

Now, $\hat{b}_{\mathbf{q}s}$ and $\hat{b}^{\dagger}_{\mathbf{q}s}$ are the annihilation operator of a phonon in the state $|\mathbf{q}, s\rangle$ and the creation operator of a phonon in the state $|\mathbf{q}, s\rangle$, respectively.

The electron-phonon interaction Hamiltonian in the complete second-quantized form can be written in a general form as

$$\hat{H}_{\rm e-ph} = \sum_{\mathbf{k}} \sum_{\zeta,\zeta'} \sum_{\mathbf{q},s} \left\{ C_{\mathbf{q}s} P^{s}_{\zeta'\zeta}(\mathbf{k},\mathbf{q}) \hat{a}^{\dagger}_{\mathbf{k}+\mathbf{q},\zeta'} \hat{a}_{\mathbf{k}\zeta} \hat{b}_{\mathbf{q}s} + C^{*}_{\mathbf{q}s} Q^{s}_{\zeta'\zeta}(\mathbf{k},\mathbf{q}) \hat{a}^{\dagger}_{\mathbf{k}-\mathbf{q},\zeta'} \hat{a}_{\mathbf{k}\zeta} \hat{b}^{\dagger}_{\mathbf{q}s} \right\}. \tag{4}$$

The factor $C_{\mathbf{q}s}$ is similar to that of the usual bulk Fröhlich Hamiltonian and

$$P^{s}_{\zeta'\zeta}(\mathbf{k},\mathbf{q}) = \langle \mathbf{k}+\mathbf{q}, \zeta' | \Phi_{\mathbf{q}s}(z) | \mathbf{k}, \zeta \rangle, \tag{5}$$

$$Q^{s}_{\zeta'\zeta}(\mathbf{k},\mathbf{q}) = \langle \mathbf{k}-\mathbf{q}, \zeta' | \Phi^{*}_{\mathbf{q}s}(z) | \mathbf{k}, \zeta \rangle. \tag{6}$$

The modulation function $\Phi_{\mathbf{q}s}(z)$ contains the effect of the presence of the interfaces along the z-direction upon the oscillations. It is, precisely, the element of distinction between this class of Hamiltonians and the bulk one, and also between themselves.

The statistical operator $\hat{w}$ and the statistical sum Ξ of the electron-phonon system, in thermal equilibrium, are given by

$$\hat{w} = \frac{1}{\Xi} e^{-\beta\hat{H}}, \tag{7}$$

$$\Xi = \mathrm{T_R} e^{-\beta\hat{H}}, \tag{8}$$

where $\beta = (k_{\rm B}T)^{-1}$ and $\mathrm{T_R}$ means the trace. Using the interaction representation and the imaginary time chronological ordering of the operators [17, 18], we may write

$$\hat{w} = \frac{1}{\Xi} e^{-\beta(\hat{H}_{\rm e}+\hat{H}_{\rm ph})} \hat{T} \exp\left\{ -\int_0^{\beta} d\tau\, \hat{H}_{\rm e-ph}(\tau) \right\}. \tag{9}$$

Let us define now the reduced statistical operator $\hat{\rho}$ of the electron subsystem trough $\hat{\rho} = \mathrm{T_{R(ph)}}\hat{w}$. Here, $\mathrm{T_{R(ph)}}$ means the trace over a complete set of states of the phonon subsystem. In order to evaluate this trace, we first define the operators

$$\hat{B}_{\mathbf{q}s}(\tau) = C_{\mathbf{q}s} \sum_{\mathbf{k},\alpha,\alpha'} P^{s}_{\zeta'\zeta}(\mathbf{k},\mathbf{q}) \hat{a}^{\dagger}_{\mathbf{k}+\mathbf{q},\alpha'}(\tau) \hat{a}_{\mathbf{k}\alpha}(\tau), \tag{10}$$

$$\hat{D}_{\mathbf{q}s}(\tau) = C^{*}_{\mathbf{q}s} \sum_{\mathbf{k},\alpha,\alpha'} Q^{s}_{\zeta'\zeta}(\mathbf{k},\mathbf{q}) \hat{a}^{\dagger}_{\mathbf{k}-\mathbf{q},\alpha'}(\tau) \hat{a}_{\mathbf{k}\alpha}(\tau), \tag{11}$$

and apply the Strukov-Fedyanin identity [19]

$$\hat{T}\exp\left\{ -\int_0^{\beta} d\tau \left[\hat{B}_{\mathbf{q}s}(\tau)\hat{b}_{\mathbf{q}s}(\tau) + \hat{D}_{\mathbf{q}s}(\tau)\hat{b}^{\dagger}_{\mathbf{q}s}(\tau) \right] \right\} = \exp\left\{ -\int_0^{\beta} d\tau \hat{D}_{\mathbf{q}s}(\tau) e^{\hbar\omega_s(\mathbf{q})\tau} \hat{b}^{\dagger}_{\mathbf{q}s} \right\} \times \exp\left\{ -\int_0^{\beta} d\tau \hat{B}_{\mathbf{q}s}(\tau) e^{-\hbar\omega_s(\mathbf{q})\tau} \hat{b}_{\mathbf{q}s} \right\} \exp\left\{ \int_0^{\beta} d\tau_1 \int_0^{\tau_1} d\tau_2 \hat{B}_{\mathbf{q}s}(\tau_1) \hat{D}_{\mathbf{q}s}(\tau_2) e^{\hbar\omega_s(\mathbf{q})(\tau_2-\tau_1)} \right\}. \tag{12}$$

The phonon operators in (12) are in the Schrödinger picture, *i.e.*, they do not depend on time. Hence, the T-operator in $\hat{\rho}$ will only order the electron operators in $\hat{B}_{\mathbf{q}s}$ and $\hat{D}_{\mathbf{q}s}$. It follows,

$$\hat{\rho} = \frac{1}{\Xi} e^{-\beta \hat{H}_e} \prod_{\mathbf{q}s} \mathrm{T}_{\mathrm{R(ph)}} \exp\left\{ -\beta\hbar\omega_s(\mathbf{q}) \hat{b}^{\dagger}_{\mathbf{q}s} \hat{b}_{\mathbf{q}s} - \hat{D}\hat{b}^{\dagger}_{\mathbf{q}s} - \hat{B}\hat{b}_{\mathbf{q}s} + \int_0^{\beta} d\tau_1 \int_0^{\beta} d\tau_2 \hat{B}_{\mathbf{q}s}(\tau_1)\hat{D}_{\mathbf{q}s}(\tau_2) e^{\hbar\omega_s(\mathbf{q})(\tau_2-\tau_1)} \right\}, \quad (13)$$

where,

$$\hat{B} = \int_0^{\beta} d\tau \hat{B}_{\mathbf{q}s}(\tau) \exp[-\hbar\omega_s(\mathbf{q})\tau], \qquad \text{and} \qquad \hat{D} = \int_0^{\beta} d\tau \hat{D}_{\mathbf{q}s}(\tau) \exp[\hbar\omega_s(\mathbf{q})\tau]. \quad (14)$$

The trace over phonon states in (13) gives

$$\mathrm{T}_{\mathrm{R(ph)}} \exp\left\{ -\beta\hbar\omega_s(\mathbf{q}) \hat{b}^{\dagger}_{\mathbf{q}s} \hat{b}_{\mathbf{q}s} - \hat{D}\hat{b}^{\dagger}_{\mathbf{q}s} - \hat{B}\hat{b}_{\mathbf{q}s} \right\} = \frac{1}{1 - e^{-\beta\hbar\omega_s(\mathbf{q})}} \exp\left[\frac{\hat{D}\hat{B}}{e^{\beta\hbar\omega_s(\mathbf{q})} - 1} \right], \quad (15)$$

and the expression for $\hat{\rho}$ becomes

$$\hat{\rho} = e^{\beta(\Omega - \hat{H}_e)} \hat{T} e^{\hat{\mathcal{V}}}, \quad (16)$$

Ω being the thermodynamical potential of the electron subsystem:

$$\Omega = -\frac{1}{\beta} \ln \mathrm{T}_{\mathrm{R}} \left[e^{-\beta\hat{H}} \hat{T} e^{\hat{\mathcal{V}}} \right]. \quad (17)$$

The operator $\hat{\mathcal{V}}$ is given by [20]

$$\hat{\mathcal{V}} = \frac{1}{2} \int_0^{\beta} d\tau_1 \int_0^{\beta} d\tau_2 \sum_{\mathbf{q}m} \sum_{\mathbf{k}_1,\mathbf{k}_2} \sum_{\zeta_1,\zeta_2} \sum_{\zeta_1',\zeta_2'} |C_{\mathbf{q}s}|^2 \Gamma(\tau_1 - \tau_2) \hat{a}^{\dagger}_{\mathbf{k}_1+\mathbf{q},\zeta_1'}(\tau_1) \hat{a}_{\mathbf{k}_1\zeta_1}(\tau_1) \hat{a}^{\dagger}_{\mathbf{k}_2-\mathbf{q},\zeta_2'}(\tau_2) \hat{a}_{\mathbf{k}_2\zeta_2}(\tau_2). \quad (18)$$

$\Gamma(\tau_1 - \tau_2)$ generically designates a function which depends on the quantum numbers $\mathbf{k}_1$, $\mathbf{k}_2$, ζ_1, ζ_1', ζ_2, ζ_2', $\mathbf{q}$, s

$$\Gamma(\tau_1 - \tau_2) = P^s_{\zeta_1'\zeta_1}(\mathbf{k}_1, \mathbf{q}) Q^s_{\zeta_2'\zeta_2}(\mathbf{k}_2, \mathbf{q}) \left[\frac{\theta(\tau_1 - \tau_2)}{1 - e^{-\beta\hbar\omega_s(\mathbf{q})}} + \frac{\theta(\tau_2 - \tau_1)}{e^{\beta\hbar\omega_s(\mathbf{q})} - 1} \right] e^{-\hbar\omega_s(\mathbf{q})(\tau_1 - \tau_2)}$$

$$+ P^s_{\zeta_2'\zeta_2}(\mathbf{k}_2, \mathbf{q}) Q^s_{\zeta_1'\zeta_1}(\mathbf{k}_1, \mathbf{q}) \left[\frac{\theta(\tau_1 - \tau_2)}{e^{\beta\hbar\omega_s(\mathbf{q})} - 1} + \frac{\theta(\tau_2 - \tau_1)}{1 - e^{-\beta\hbar\omega_s(\mathbf{q})}} \right] e^{\hbar\omega_s(\mathbf{q})(\tau_1 - \tau_2)}. \quad (19)$$

Expressions (16)–(19) resume the reduction of the electron-phonon system to an electronic one. In this system any pair of electrons interact through a retarded potential given by $\hat{\mathcal{V}}$. The statistical average of any operator is evaluated by using the reduced statistical operator $\hat{\rho}$ and every elementary act of interaction may be represented by a term of the form

$$|C_{\mathbf{q}s}|^2 \Gamma(\tau_1 - \tau_2) \hat{a}^{\dagger}_{\mathbf{k}_1+\mathbf{q},\zeta_1'}(\tau_1) \hat{a}_{\mathbf{k}_1\zeta_1}(\tau_1) \hat{a}^{\dagger}_{\mathbf{k}_2-\mathbf{q},\zeta_2'}(\tau_2) \hat{a}_{\mathbf{k}_2\zeta_2}(\tau_2) :$$

At the time τ_2, an electron with quantum numbers $\mathbf{k}_2, \zeta_2$ annihilates and another electron with wavevector $\mathbf{k}_2 - \mathbf{q}$ and quantum number ζ_2' (not necessarily equals to ζ_2) is created. The transferred momentum $\hbar\mathbf{q}$ and energy propagate with the field until instant τ_1 when they are absorbed by another electron. The second scattering process involves the annihilation of an electron in the state $|\mathbf{k}_1 + \mathbf{q}, \zeta_1'\rangle$. This electron-electron interaction through the crystal lattice is also applied to the electron self-interaction, *i.e.*; the excitation created at τ_2 (expressed in terms of phonon emission and absorption) propagates in the lattice and acts upon the same electron at time τ_1.

At this point, it should be remarked that the reduction of the electron-phonon interaction to an effective electron-electron one, obtained along the lines of the procedure above developed is an exact result. No approximation has been performed when summing over phonon variables with the use of identity (12), except for the general assumption that the electron-phonon interaction Hamiltonian is Fröhlich-like.

3. The one-electron Green's function and the thermodynamical potential

The one-particle Green's function in the interaction representation is given by [17, 18]

$$G(\mathbf{k}, \zeta; \tau) = -\frac{\langle \hat{T}\{\hat{a}_{\mathbf{k}\zeta}(\tau) \hat{a}^{\dagger}_{\mathbf{k}\zeta}(0) e^{\hat{\mathcal{V}}}\}\rangle_0}{\langle \hat{T}\{e^{\hat{\mathcal{V}}}\}\rangle_0}. \quad (20)$$

Here, the average is performed with the use of the statistical operator of the non-interacting electron subsystem. Wick's

theorem can be applied and, as usual, the contribution of disconnected terms cancels with the denominator, resulting in

$$G(\mathbf{k},\zeta;\tau) = \sum_{n=0}^{\infty} G^{(n)}(\mathbf{k},\zeta;\tau), \tag{21}$$

where

$$G^{(n)}(\mathbf{k},\zeta;\tau) = -\frac{1}{n!}\langle \hat{T}\{\hat{a}_{\mathbf{k}\zeta}(\tau)\hat{a}^{\dagger}_{\mathbf{k}\zeta}(0)\hat{\mathcal{V}}^{n}\}\rangle_{0}^{\mathrm{con}}. \tag{22}$$

Now, following the standard procedure of Ref. 17, if

$$\Omega_{\mathrm{e}} = -\frac{1}{\beta}\ln \mathrm{Tr}e^{-\beta\hat{H}_{\mathrm{e}}} \tag{23}$$

is the thermodynamical potential corresponding to the non-interacting electron subsystem, the correction $\Delta\Omega = \Omega - \Omega_e$ associated to the electron-phonon interaction will be given by

$$\Delta\Omega = -\frac{1}{\beta}\left\{\langle \mathrm{Tr}e^{\hat{\mathcal{V}}}\rangle_{0}^{\mathrm{con}} - 1\right\}. \tag{24}$$

In all Fröhlich-like problems, the expansion of $e^{\hat{\mathcal{V}}}$ can be viewed as a series in the electron-phonon coupling constant α, in such a way that the n-th order term in the expansion for the Green's function is proportional to the n-th power of α. This feature allows us to write

$$\Delta\Omega = \frac{1}{\beta}\int_{0}^{\alpha}\frac{d\alpha}{\alpha}\sum_{\mathbf{k},\zeta}\left\{\frac{G(\mathbf{k},\zeta;\tau)}{G^{(0)}(\mathbf{k},\zeta;\tau)} - 1\right\}, \tag{25}$$

thus expressing through the one-electron Green's function the correction to the electronic thermodynamical potential due to the interaction with the phonons. From (25) it can be derived the usual series of "bubble" diagrams corresponding to this quantity [17, 18].

4. Polaron free energy in a GaAs/AlAs double heterostructure

In this section, the many-body approach developed in Secs. 2 and 3 will be applied to the calculation of the polaron energy in a GaAs/AlAs double heterostructure (DHS) for both zero and finite temperature. This is going to be done within the framework of the DECM for the long-wavelength polar optical phonons [14]. The GaAs-like phonon modes are neither purely confined slab modes nor interface modes. There is a mixed character and certain modes are rather more interface-like than the others. Furthermore, we only can say that the modes may be predominantly "longitudinal" (quasi-L) in some cases or predominantly "transversal" (quasi-T) in others because the polarization also exhibits a mixed character. The corresponding electron-phonon interaction Hamiltonian is

$$\hat{H}_{\mathrm{e-ph}} = \sum_{\mathbf{k},\zeta',\zeta}\sum_{\mathbf{q},m} C_{\mathbf{q}m}P^{m}_{\zeta'\zeta}(\mathbf{k},\mathbf{q}) \times \left(\hat{a}^{\dagger}_{\mathbf{k}+\mathbf{q},\zeta'}\hat{a}_{\mathbf{k}\zeta}\hat{b}_{\mathbf{q}m} + \hat{a}^{\dagger}_{\mathbf{k}-\mathbf{q},\zeta'}\hat{a}_{\mathbf{k}\zeta}\hat{b}^{\dagger}_{\mathbf{q}m}\right), \tag{26}$$

where $m = 1, 2, \ldots$, labels the set of discrete optical phonon modes which appear due to the presence of the interfaces and ζ', ζ label the different electronic states in the well. The factor $C_{\mathbf{q}m}$ is given by,

$$C_{\mathbf{q}m} = \left[\frac{4\pi\hbar e^{2}(\omega^{2}_{\mathrm{TO}} - \omega^{2}_{\mathrm{LO}})}{\epsilon_{\infty}\omega_{m}(\mathbf{q})Sd}\right]^{1/2}. \tag{27}$$

Here, S is the transverse area, d is the well width, and ϵ_{∞}, ω_{TO} and ω_{LO} are, respectively, the high frequency dielectric constant, the frequency of the tranversal optical phonons and the frequency of the longitudinal optical phonons in the bulk GaAs. $\omega_m(\mathbf{q})$ are the characteristic dispersion relations of the different oscillation modes [16, 21].

On the other hand,

$$P^{m}_{\zeta'\zeta}(\mathbf{k},\mathbf{q}) = \langle \mathbf{k}+\mathbf{q},\zeta'|f_{\mathbf{q}m}(z)|\mathbf{k},\zeta\rangle. \tag{28}$$

$f_{\mathbf{q}m}$—the electrostatic potential—is a real function which depends only on $|\mathbf{q}|$. If the quantum well is chosen to be symmetric with respect to $z = 0$, the function $f_{\mathbf{q}m}$ will represent either odd potential states or even potential states for the phonons [21].

The conduction band electronic states in the GaAs/AlAs DHS are calculated using a finite barrier quantum-well model, explicitly considering the difference between the effective masses in both materials (see Ref. 22, for instance). The barrier height is taken to be $V_0 = 915$ meV. Additionally, it will be also assumed that the electron is in the Γ band even when it is really the X the lowest conduction band. This is done mostly for two reasons. The first one is that we are interested in the dynamics around $\mathbf{k}$=0 in the well because the interaction with mechanically confined GaAs-like phonon modes should participate more strongly in the renormalization effect of the bottom of the conduction band in this material. The use of the barrier height corresponding to the X point in AlAs (567 meV) would not actually represent that situation. The second reason is of much more practical character: to avoid the extra complication coming from the consideration of an indirect gap, and it has been taken into account in previous works as well [23].

In a finite barrier model quantum well, to sum over all intermediate states is a less practicable process. However, If we are interested, for instance, in polaron corrections to the first subband ($\zeta = 1$) energy, taking only the very first terms in the summation is enough for the numerical evaluation and, in most cases, keeping only the contribution from the first excited level ($\zeta = 2$) will do. This second contribution is higher for wider quantum wells where first and second subbands are closer and the combined thermal and optical-phonon energies result to be $\hbar\omega_m(q) + k_{\mathrm{B}}T \geq \varepsilon_2 - \varepsilon_1$, thus giving the possibility of a more intense intersubband scattering process.

The evaluation of (28) leads to the following function for the square matrix elements:

$$I_{11}^{m}(q) = A_m^2(q)\left(\frac{2\kappa\kappa_b}{\kappa + 2\kappa\kappa_b + \kappa\cos 2\kappa + \kappa_b \sin 2\kappa}\right)^2 \left\{ \frac{2\kappa \sin 2\kappa}{4\kappa^2 - k_L^2}\cos k_L + k_L\left(\frac{1}{k_L^2} - \frac{\cos 2\kappa}{4\kappa^2 - k_L^2}\right)\sin k_L \right.$$
$$\left. - \frac{C_L}{\xi}e^{-\xi}\left[\frac{2\kappa \sin 2\kappa}{4\kappa^2 + \xi^2}\cosh\xi + \left(\frac{\xi\cos 2\kappa}{4\kappa^2 + \xi^2} + \frac{1}{\xi}\right)\sinh\xi\right] + 2C_0 e^{-(\xi + 2\kappa_b)}\frac{\cos^2\kappa}{2\kappa_b + \xi}\right\}^2;$$

$$I_{12}^{m}(q) = B_m^2(q)\left(\frac{2\kappa\kappa_b}{\kappa + 2\kappa\kappa_b + \kappa\cos 2\kappa + \kappa_b \sin 2\kappa}\right)\left(\frac{2\eta\eta_b}{\eta + 2\eta\eta_b - \eta\cos 2\eta - \eta_b \sin 2\eta}\right)$$
$$\times \left[\frac{\sin(\kappa + \eta - k_L)}{\kappa + \eta - k_L} + \frac{\sin(\kappa - \eta + k_L)}{\kappa - \eta + k_L} + \frac{\sin(\kappa + \eta + k_L)}{\kappa + \eta + k_L} - \frac{\sin(\kappa - \eta - k_L)}{\kappa - \eta - k_L}\right.$$
$$- S_L\left\{(1 + e^{2\xi})\left[\frac{\sin(\kappa + \eta)}{\xi^2 + (\kappa + \eta)^2} + \frac{\sin(\eta - \kappa)}{\xi^2 + (\eta - \kappa)^2}\right]\right.$$
$$\left.\left. - (1 - e^{-2\xi})\left[\frac{\kappa + \eta}{\xi}\frac{\cos(\kappa + \eta)}{\xi^2 + (\kappa + \eta)^2} + \frac{\eta - \kappa}{\xi}\frac{\cos(\eta - \kappa)}{\xi^2 + (\eta - \kappa)^2}\right]\right\} + 2S_0\frac{\sin\eta\cos\kappa}{\xi + \kappa_b + \eta_b}e^{-(\xi + \kappa_b + \eta_b)}\right]^2 \tag{29}$$

In the former expressions, the quantities $\xi = qd/2$, $\kappa = \sqrt{(m^* d^2/2\hbar^2)\varepsilon_1}$, $\kappa_b = \sqrt{(m_b^* d^2/2\hbar^2)(V_0 - \varepsilon_1)}$, $\eta = \sqrt{(m^* d^2/2\hbar^2)\varepsilon_2}$, and $\eta_b = \sqrt{(m_b^* d^2/2\hbar^2)(V_0 - \varepsilon_2)}$ have been introduced; ε_1 (ε_2) being the energy of the first (second) level in the quantum well, m^* the conduction band effective mass of the GaAs, and m_b^* the Γ-point conduction band effective mass of the AlAs. The quantity k_L is given by

$$k_L = \frac{d}{2}\sqrt{\frac{\omega_{\mathrm{LO}}^2 - \omega_m^2(q)}{\beta_L^2} - q^2},$$

with $\beta_L = 3.2 \times 10^5$ cm/s, and

$$C_L = \xi\cos k_L - k_L \sin k_L;$$

$$S_L = \xi \sin k_L + k_L \cos k_L;$$

$$C_0 = \cos k_L \sinh\xi + \frac{k_L}{\xi}\sin k_L \cosh\xi;$$

$$S_0 = \sin k_L \cosh\xi - \frac{k_L}{\xi}\cos k_L \sinh\xi. \tag{30}$$

Finally, A_m is certain q-dependent normalization constant for the even potential oscillation modes, and B_m is the corresponding nomalization constant in the case of the oscillation modes with odd electrostatic potential [16, 21].

Starting from the Eq. (25), with the use of (27), and taking the one-electron limit, it is possible to write for the first-order polaron free energy correction in the DHS, the following expression:

$$F^{(1)}(t) = -\frac{4\alpha\hbar\omega_{\mathrm{LO}}R}{d}\frac{e^{-\beta\varepsilon_1}}{\sum_j e^{-t\varepsilon_j/\hbar\omega_{\mathrm{LO}}}}\sum_m\sum_{l=1,2}\int_0^\infty dq\frac{qI_{11}^m(q)}{\omega_{qm}}\int_0^{t/2} dx e^{-\Delta_{l1}x}D_{qm}(x)e^{-q^2R^2x(1-\frac{x}{t})}; \tag{31}$$

where $t = \hbar\omega_{\mathrm{LO}}\beta$ is a dimensionless temperature-dependent variable and $\omega_{qm} = \omega_m(q)/\omega_{\mathrm{LO}}$. $\Delta_{l1} = (\varepsilon_l - \varepsilon_1)/\hbar\omega_{\mathrm{LO}}$, and $R = (\hbar/2m^*\omega_{\mathrm{LO}})^{1/2}$ is the bulk polaron radius. The summation over index j comes from the quasi-2D expression for the exponential $e^{\beta\mu}$. Again, it is restricted to go over the discrete energy levels of the well. The function $D_{mq}(x)$ is—according to (19)—

$$D_{qm}(x) = \frac{e^{\omega_{qm}x}}{e^{\omega_{qm}t} - 1} + \frac{e^{-\omega_{mq}x}}{1 - e^{-\omega_{qm}t}}. \tag{32}$$

The integration over the variable x can be performed and expressed through the error function integral

$$\int_0^x e^{a^2x^2}dx = \frac{\sqrt{\pi}}{2a}\,\mathrm{erfi}\,(ax),$$

thus allowing to write

$$F^{(1)}(t) = -\frac{2\alpha\sqrt{\pi t}\hbar\omega_{\rm LO}}{d\sum_j e^{-t\varepsilon_j/\hbar\omega_{\rm LO}}} \sum_m \sum_{l=1,2} \int_0^\infty dq \frac{I_{11}^m(q)}{\omega_{qm} t} \left\{ \frac{\exp\left[-(q^2R^2 + \Delta_{l1} - \omega_{qm})\right]}{\exp(\omega_{qm}) - 1} \right.$$
$$\times \left[\mathrm{erfi}\left(\frac{q^2R^2 + \Delta_{l1} - \omega_{qm}}{2qR}\sqrt{t} \right) + \mathrm{erfi}\left(\frac{\omega_{qm} - \Delta_{l1}}{2qR}\sqrt{t} \right) \right]$$
$$\left. + \frac{\exp\left[-(q^2R^2 + \Delta_{l1} + \omega_{qm})\right]}{1 - \exp(-\omega_{qm}t)} \left[\mathrm{erfi}\left(\frac{q^2R^2 + \Delta_{l1} + \omega_{qm}}{2qR}\sqrt{t} \right) - \mathrm{erfi}\left(\frac{\omega_{qm} + \Delta_{l1}}{2qR}\sqrt{t} \right) \right] \right\}. \quad (33)$$

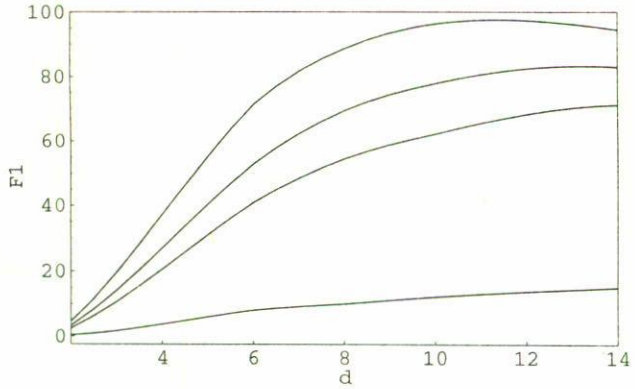

FIGURE 1. Relative polaron free energy as a function of the GaAs quantum well width (in nanometers). Curves, in decreasing order, correspond respectively to 613 K, 420 K, 300 K, and 0 K.

In the calculations, the values $\omega_{\rm LO} = 291.9$ cm^{-1}; $\omega_{TO} = 273.8$ cm^{-1}; $\epsilon_0 = 13.18$; $\epsilon_\infty = 10.89$; $m^* = 0.0665\, m_0$, and $\alpha = 0.068$ were taken for GaAs. For the well barrier effective mass we used m^*(AlAs)$= 0.15\, m_0$, m_0 being the bare electron mass.

In Fig. 1 the relative polaron free-energy Fr is shown as a function of the quantum well width d for different values of the temperature. Fr is defined as the ratio $F^{(1)}(t)/F_{\rm 3D}^{(1)}(t)$; where $F_{\rm 3D}^{(1)}(t)$, the polaron free-energy in first order for bulk GaAs is given by:

$$F_{\rm 3D}^{(1)}(t) = -\frac{\alpha\hbar\omega_{\rm LO}}{\sqrt{\pi}}\sqrt{t}\int_0^{t/2} dx \frac{D(x)}{\sqrt{x(t-x)}} \quad (34)$$

where

$$D(x) = \frac{e^x}{e^t - 1} + \frac{e^{-x}}{1 - e^{-t}}. \quad (35)$$

In the limit $T = 0$ K ($t = \infty$), equation (35) gives precisely the bulk polaron binding energy value $-\alpha\hbar\omega_{\rm LO}$ [18].

The three upper curves in the figure correspond, from top to bottom, to the Debye temperature of the GaAs ($T_D = 613$ K), the LO-phonon temperature of the material ($T_{\rm ph} = \hbar\omega_{\rm LO}/k_{\rm B} = 420$ K), and to $T = 300$ K, respectively. Besides the room temperature value, the other two were chosen because they constitute significative temperatures for the material. For the sake of comparison, a lowest curve, corresponding to the $T = 0$ K polaron relative binding energy has been included. This curve is obtained from the expression resulting when taking the limit $t \to \infty$ of Eq. (32), which precisely coincides with the Rayleigh-Schrödinger-perturbation-theory equation presented in Ref. 22.

As expected, the polaron free energy raises with increasing quantum well width. The rate of increment varies for different temperatures indicating that the way by which the GaAs-like phonon modes contribute depends on the temperature as well. Nevertheless, it can be observed a tendency to change the monotony, which reverses towards a limiting bulk-value for d sufficiently large. This decreasing behavior is stronger at high temperatures—as it is shown in the curve corresponding to T_D—, while is much more subtle for $T = 0$ K. The range of well width values selected represents the region of greater interest for the effect here studied. Furthermore, there exists another reason -this time of practical character: for higher values of d, the number of eigenmodes associated to the characterictics equations increases very rapidly, and the calculation process becomes really tedious [16, 21, 22].

Relative polaron free energy is not reported for d below 2 nm for in that region a macroscopic continuum model for the GaAs long-wavelength oscillations would certainly not work well, and its validity is doubtful. When $d \to 0$, only the bulk AlAs is present. However, in this study we have not considered so far the contribution to the electron-phonon interaction coming from the electric potential of the barrier modes. If taken into account, it will significatively change (by increasing) the polaronic correction for the smallest values of d; but in the case of well width around 10 nm and beyond the main contribution should come from GaAs-like polar optical modes.

5. Conclusions

We have presented a new formalism for a many-body treatment of the electron-phonon interaction in semiconductor layered heterostructures. The simplest application of this formalism is the study of the polaron properties. We chose, as a particular case, a model derived in Refs. 16 and 21 for the polar optical oscillations in a GaAs/AlAs DHS. The results obtained within this model indicate that the effect of the modification of the phonon spectrum due to the existence of interfaces is relevant only for layer thickness not too larger than

100 angstroms. Significant differences with the 3D values are obtained for a GaAs-layer width of a few tens of angstroms. For wide enough wells, the use of the bulk Fröhlich Hamiltonian would provide good results.

In our opinion, the advantage of the reduction of the electron-phonon interaction to an effective electron-electron one could be of interest when studying the many-electron system in heterostructures—including both the Coulomb interaction and that with the phonons—, as well as for the study of another properties like the electronic mobility, by using the Kubo formula [18]. As it was already mentioned in Sec. 1, the formalism can be adapted in straightforward manner to deal with the electron-phonon interaction in other planar heterostructures as well as in quasi-one- and quasi-cero-dimensional semiconducting systems provided the interaction Hamiltonian can be written—in the $\hat{a}$ and $\hat{b}$ operators—in a form isomorphic with Eq. (4); *i.e.* a Fröhlich-like Hamiltonian.

On the other hand, the very structure of the identity expressed through Eq. (12) could allow for a similar summation procedure in another kinds of interaction; *e.g.* the phonon-magnon problem, provided a finite temperature perturbative Green's function formalism could be applied to.

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