Electron–confined-phonon interaction in quantum wells: Reformulation of the slab model

Gerald Weber*

Departamento de Física, Instituto de Ciências Exatas, Universidade Federal de Minas Gerais, Caixa Postal 702, 30161-970 Belo Horizonte, Minas Gerais, Brazil

(Received 26 May 1992)

We show that the Fuchs-Kliewer slab model, as used for the description of the electron-phonon Fröhlich interaction in quantum wells and superlattices, can be reformulated in a simple way and it becomes very close to the Huang and Zhu model, based on a lattice-dynamic approach. This simple reformulation answers several questions which have been made over the past few years about the dielectric continuum model, especially those about the existence of a half-wavelength mode of the z component of the relative ionic displacement which has no counterpart in microscopic calculations. We show that in fact this mode does not exist in the reformulated slab model.

The dielectric continuum model is an attractive method to study scattering due to electron-phonon (Fröhlich) interactions in low-dimensional structures such as semiconductor quantum wells and superlattices. Several device properties such as mobilities, relaxation rates, and phonon-assisted tunneling currents can be calculated without too much effort in this way.

The first theory, originally developed for dielectric slabs of relatively large dimensions (several μm),[1–4] was recently adapted for the use in quantum wells and is usually referred to as the Fuchs-Kliewer slab model or simply the slab model. Discrepancies between microscopic lattice-dynamic calculations and these models gave origin to an intense debate about the validity of this theory (for a review see Menéndez[5] and Cardona[6]). Some authors[7–10] proposed the use of different boundary conditions (hydrodynamic boundary conditions) arguing that the continuity of the z component of the mechanical relative displacement has a greater importance than the parallel component (which is proportional to the phonon potential) due to the predominantly mechanical nature of LO modes.[11] This alternative description, frequently referred to as the guided modes model, results in smaller scattering rates for intrasubband transitions and larger scattering rates for intersubband transitions. Recently, Rücker, Molinari, and Lugli[12] pointed out that the results of the guided modes model are inconsistent with scattering rates obtained from microscopic calculations, therefore this model is being increasingly ruled out as a valid alternative to the Fuchs-Kliewer slab model.

Huang and Zhu[13] proposed an *ad hoc* model based on a lattice-dynamic calculation, which reproduces closely their results of microscopic calculations. Comparing the Huang and Zhu model with the slab model, as derived by Fuchs and Kliewer,[1] it is found that a half-wavelength mode of the z component of the relative ionic displacement u_z, which is present in the Fuchs-Kliewer slab model, is absent in the microscopic calculation and hence in the Huang and Zhu model. Huang and Zhu argued that this mode should correspond to an interface mode obtained in the microscopic theory, when dispersion is taken into account.[13,14] We will show in this Brief Report that this half-wavelength mode of u_z in fact does not exist in the reformulated slab model.

The Huang and Zhu model has received a large acceptance and is believed to be the dielectric continuum model (although *ad hoc* in nature) which currently best describes the electron-phonon interaction in quasi-two-dimensional systems.

The modes *presently* obtained from the Fuchs-Kliewer slab model are the result of a wrongly defined arbitrary function. When a correctly defined arbitrary function is used a different set of independent solutions is obtained which are very close to the phenomenological form proposed by Huang and Zhu.[13]

We now present a brief description of the differential equation which leads to the solutions of the relative ionic displacements, essential for the derivation of the electron-phonon interaction Hamiltonian, of the slab model. For more details on this theory we refer the reader to Refs. 1 and 4.

For the case of a dielectric slab, the Maxwell equations in the limit of no retardation will result in the following differential equation for the phonon potential:[2,4]

$$\epsilon(\omega)\left(\frac{\partial^2}{\partial z^2}-q_{\parallel}^2\right)\phi(z)=0. \tag{1}$$

Note that at the bulk LO-phonon frequency the dielectric function in the slab is zero $\epsilon(\omega_{\rm LO}^{\rm bulk})=0$, therefore any arbitrary electric field satisfies Eq. (1). The only constraint now is the electrodynamic boundary condition to be applied on the electric fields. Ouside the slab [where $\epsilon(\omega)\neq 0$] Eq. (1) has as solutions exponential decaying functions. With the boundary conditions applied on the electric field $\mathbf{E}$ and the displacement field $\mathbf{D}$ (Ref. 15) we obtain that the phonon potential outside the slab has to vanish.[4]

At frequencies lying within the limit of the bulk phonon frequencies, i.e., between $\omega_{\rm LO}^{\rm bulk}$ and $\omega_{\rm TO}^{\rm bulk}$, the dielectric function is not zero in the slab and the potential $\phi(z)$ must satisfy the differential equation [Eq. (1)]; thus the well-known interface phonons are obtained.

The interface phonons are now well understood from a theoretical as well as from an experimental point of view. Remaining disagreements concern mainly the confined phonon modes. Let us study, for instance, the properties of an arbitrary function $f(x)$ expanded over a complete set of orthogonal functions. The standard Fourier series in the interval $[-\pi,\pi]$ is such a function,

$$f(x) = \frac{a_0}{2} + \sum_{j=1}^{\infty}[a_j \cos(jx) + b_j \sin(jx)]. \tag{2}$$

In the dielectric continuum theory, as derived by Licari and Evrard,[4] the phonon potential is zero outside the slab, therefore we seek $f(\pm\pi) = 0$ which enables us to eliminate the coefficient a_0 and obtain

$$f(x) = \sum_{j=1}^{\infty} \left\{a_j \left[\cos(jx) - (-1)^j\right] + b_j \sin(jx)\right\}. \tag{3}$$

We now perform a change of indexes in the following way: $j = k/2$ for the cosine series and $j = (k+1)/2$ for the sine series,

$$f(x) = \sum_{k=1}^{\infty} \begin{cases} A_k \left[\cos(kx/2) - (-1)^{k/2}\right], & k = 2,4,6,\ldots \\ B_k \sin(k+1)x/2, & k = 1,3,5,\ldots \end{cases} \tag{4}$$

i.e., labeling the even-parity modes $[f_k(x) = f_k(-x)]$ with even indexes and odd-parity modes $[f_k(x) = -f_k(-x)]$ with odd indexes, without loss of generality. Within the framework of the dielectric continuum model (we follow closely the delevopment of Sec. III of the work by Licari and Evrard[4]), we can then derive a phonon potential function for the confined phonons,

$$\phi_n(z) = \begin{cases} a_n \sin[(n+1)z\pi/L], & n = 1,3,5,\ldots \\ b_n \cos(nz\pi/L) - (-1)^{n/2}, & n = 2,4,6,\ldots \end{cases} \tag{5}$$

where a_n and b_n are constants. Note that the phonon potential $\phi(z)$ is proportional to the parallel component of the relative ionic displacement $u_{\|}(z)$, and its derivative is proportional to the z component $u_z(z)$.

Note that the even modes in Eq. (5) are *exactly* the same as in the Huang and Zhu model,[13]

$$\phi_{n'}^{\mathrm{HZ}}(z) = \begin{cases} a_{n'} \sin(\mu_{n'}\pi z/L) + C_{n'} z/L, & n' = 3,5,7,\ldots \\ b_{n'} \cos(n'z\pi/L) - (-1)^{n'/2}, & n' = 2,4,3,\ldots \end{cases} \tag{6}$$

where we have used the label n' to distinguish from the labeling used in Eq. (5).

In order to compare Eqs. (5) and (6) directly we use $n' = n+2$ for odd modes and $n' = n$ for even modes. At a first glance the odd modes in the reformulated slab model and in the Huang and Zhu model seem to be very different. Yet at a closer inspection it becomes evident that this is not the case as Fig. 1 illustrates.

If we compare the reformulated slab model with the original Fuchs-Kliewer model we notice that only the even-parity modes have changed in the reformulation, the odd-parity modes remain unaltered. This may not be immediately clear due to the different labeling used in this reformulation. Although it is generally agreed[5] that the labeling in the slab model is arbitrary due to the degeneracy of the modes, it is nevertheless convenient that the labeling reflects the parity of the phonon potential function.

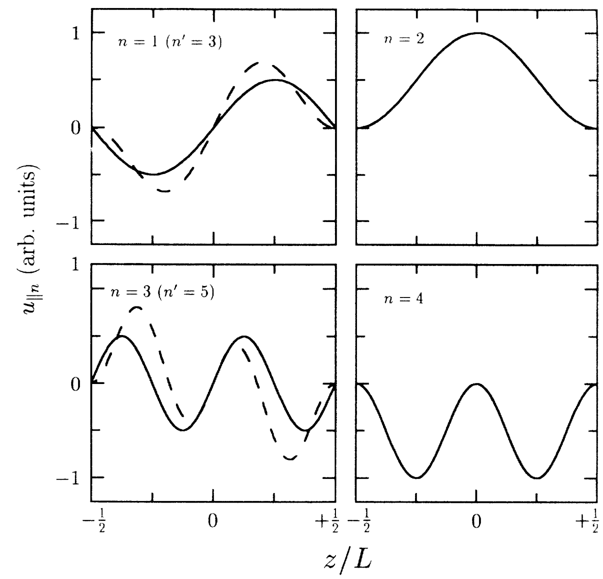

FIG. 1. Parallel components of the confined-phonon relative ionic displacements $u_{\|}$ [proportional to the phonon potential $\phi(z)$] for the reformulated slab model (full curves) and for the Huang and Zhu model (dashed curves).

Figure 2 shows the z component of the relative ionic displacement for the reformulated slab model and the Huang and Zhu model. The half-wavelength mode, present in the original slab model, is absent in the reformulated slab model.

It is now clear, from the discussion above and from Fig. 2, that the absent $n' = 1$ mode in the Huang and Zhu model is not a half-wavelength confined mode which has become an interface mode under given circumstances (hybridization), because this mode simply does not exist. As Eq. (5) is a complete set of solutions it is unlikely that there is any important mode missing from the model of Huang and Zhu. It is not surprising, therefore, that the scattering rates obtained for the odd-parity modes are almost indistinguishable from those calculated for the Fuchs-Kliewer slab model[16] even when a uniform longitudinal electric field is applied.[17] Rudin and Reinecke initially found significant differences in the scattering rates[18] between the Fuchs-Kliewer slab model and the Huang and Zhu model, but corrected their calculation afterwards[19] and now also show that this difference is very small indeed. It would be expected that the absence of a fundamental mode should result in important changes in scattering rates, which has not been the case. Notice that we are not ruling out the mixing of

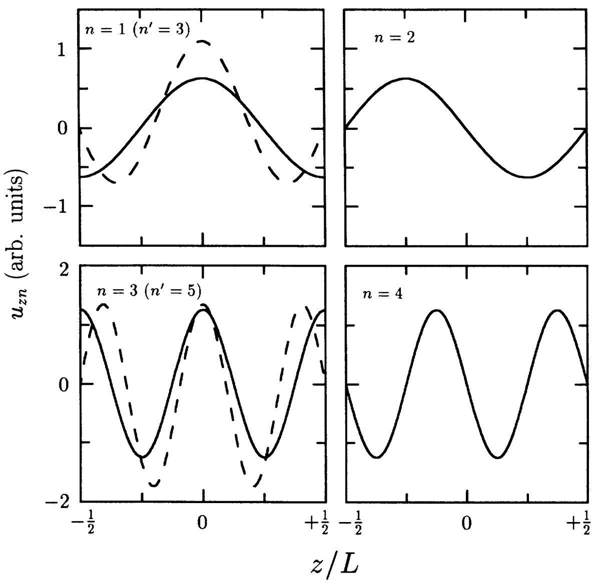

FIG. 2. z component of the confined-phonon relative ionic displacement u_z for the reformulated slab model (full curves) and for the Huang and Zhu model (dashed curves). Note u_z is proportional to the first derivative of the parallel component $u_{\parallel}$, shown in Fig.1.

confined and interface modes (hybridization) which is a completely different issue.

Recently, Zianni, Butcher, and Dharssi[20] introduced a parabolic bulk phonon-dispersion relation into the phenomenological equations of Born and Huang[11] in order to obtain confined-phonon potentials. In the dispersionless limit they found confined-phonon potential functions similar to the Huang and Zhu model. One should expect to obtain, in the dispersionless limit, the potential functions of the original Fuchs-Kliewer slab model, which is not the case as shown in Ref. 20. This can be regarded as additional evidence of the correctness of our reformulation.

We have shown, using a very simple Fourier-series analysis, that the confined modes in the slab model take a different form from the one initially assumed by Fuchs and Kliewer.[1] Once reformulated, the slab model turns out to be very similar to the Huang and Zhu model, and recent works by other groups[20] seem to provide further evidence of the correctness of our results. In particular, we found that it is unlikely that there is any mode absent from the Huang and Zhu model; the only major problem of this model seems to be the nonorthogonality of the phonon potentials. This issue was recently treated by Haupt and Wendler[21] who orthonormalized the phonon modes of the Huang and Zhu model. Our reformulation also explains the striking similarity of intersubband scattering rates obtained by this model and the Huang and Zhu model.[16,19]

In conclusion, our simple reformulation provides an answer to many questions raised about the original slab model since its first publications by Fuchs and Kliewer 27 years ago. We believe that the slab model has now been shifted into a coherent picture.

We are grateful to A. M. de Paula for helpful discussions. Financial support by Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) is acknowledged.

*Electronic address: gweber@brufmg (Bitnet)

[1] R. Fuchs and K. L. Kliewer, Phys. Rev. **140**, A2076 (1965).
[2] A. A. Lucas, E. Kartheuser, and R. G. Badro, Phys. Rev. B **2**, 2488 (1970).
[3] V. V. Bryksin and Y. A. Firsov, Sov. Phys. Solid State **13**, 398 (1971).
[4] J. J. Licari and R. Evrard, Phys. Rev. B **15**, 2254 (1977).
[5] J. Menéndez, J. Lumin. **44**, 285 (1989).
[6] M. Cardona, Superlatt. Microstruct. **5**, 27 (1989).
[7] M. Babiker, J. Phys. C **19**, 683 (1986).
[8] B. K. Ridley, Phys. Rev. B **39**, 5282 (1989).
[9] B. K. Ridley, Rep. Prog. Phys. **54**, 169 (1991).
[10] B. K. Ridley and M. Babiker, Phys. Rev. B **43**, 9096 (1991).
[11] M. Born and K. Huang, *Dynamical Theory of Crystal Lattices* (Clarendon, Oxford, 1954).
[12] H. Rücker, E. Molinari, and P. Lugli, Phys. Rev. B **44**, 3463 (1991).
[13] K. Huang and B. Zhu, Phys. Rev. B **38**, 13 377 (1988).
[14] K. Huang and B.-F. Zhu, Phys. Rev. B **38**, 2183 (1988).
[15] J. D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1962).
[16] G. Weber, A. M. de Paula, and J. F. Ryan, Semicond. Sci. Technol. **6**, 397 (1991).
[17] G. Weber and J. F. Ryan, Phys. Rev. B **45**, 11 202 (1992).
[18] S. Rudin and T. L. Reinecke, Phys. Rev. B **41**, 7713 (1990).
[19] S. Rudin and T. L. Reinecke, Phys. Rev. B **43**, 9298(E) (1991).
[20] X. Zianni, P. N. Butcher, and I. Dharssi, J. Phys. Condens. Matter **4**, L77 (1992).
[21] R. Haupt and L. Wendler, Phys. Rev. B **44**, 1850 (1991).