On polar optical vibrational quantum excitations in semiconductor nanostructures

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By applying a phenomenological treatment of long-wavelength polar optical oscillations in semiconductor nanostructures we derive a general approximated expression for the energy spectrum of the elementary excitations that depends essentially on the nanostructure geometry.

Keywords: Polar optical oscillations; elementary excitations in nanostructures

Aplicando un modelo fenomenológico de oscilaciones óptico-polares de onda larga en nanoestructuras semiconductoras, se deriva una expresión general aproximada para el espectro energético de las excitaciones elementales. Dicho espectro depende de manera esencial de la geometría de la nanoestructura.

Descriptores: Oscilaciones óptico-polares; excitaciones elementales en nanoestructuras

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1. Introduction

Polar optical vibrations in semiconductor nanostructures (SNS's) of the type of quantum wells [1–8], quantum wires [9], quantum dots [10–12], and superlattices [13], have been intensively investigated in the last years. Several advanced techniques have permitted the growth of such low-dimensional systems that possess important physical properties suggesting a broad spectrum of device applications. Therefore, the energy spectrum and optical properties in SNS's are submitted to extensive studies. Important role in many physical processes play the polar optical oscillations, especially in the long-wavelength limit. Several theoretical treatments for long-wavelength oscillations based on phenomenological continuum approach or involving microscopic numerical calculations may be met in previous works [14–20].

Recently C. Trallero-Giner *et al.* [21, 22] have proposed a phenomenological approach to long-wavelength polar optical phonons in SNS's. They postulated, in the spirit of the classical theory of macroscopic media the following Lagrangian density:

$$\mathcal{L} = \frac{1}{2}\rho \cdot \left|\frac{\partial \vec{u}}{dt}\right|^2 - \frac{1}{2}\rho\omega^2\vec{u}^2 - \alpha \cdot \vec{u}\,\nabla\phi + \frac{1}{8\pi}\varepsilon_\infty|\nabla\phi|^2 + \frac{1}{2}\lambda_{ijkl}u_{ij}u_{kl}, \quad (1)$$

which takes into account phonon dispersion up to quadratic terms in the wave vector, as well as the coupling between the electrostatic potential ϕ and the mechanical vibration displacement $\vec{u}$.

Considering the Lagrangian density (1), they obtained the equations of motion and solved it within a given homogeneous part of the structure and applying suitable boundary-matching conditions at the interfaces. In this work, we have interested in the study of the energy spectrum of the long-wavelength polar optical vibrations in SNS's characterizing the field represented by (1).

2. Brief review of the model

We assume a material with isotropic dielectric response and vibrational dispersion relation. The oscillations are described by the displacement vector field $\vec{u}$ that represents the relative displacement of the two ions involved. The electric potential ϕ is related with the electric field by $\vec{E} = -\nabla\phi$, corresponding to a quasistationary treatment of Maxwell equations in the unretarded limit ($c \to \infty$). The internal stresses of the medium are incorporated in the fifth term of (1) through the strain tensor:

$$u_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \quad (2)$$

and the tensor λ_{ijkl} closely related to the elastic moduli tensor [23, 24]. This term results relevant in SNS's because it gives the possibility to introduce boundary-matching conditions for $\vec{u}$ at the interfaces. At the same time it leads to dispersive oscillations. Other physical parameters of the medium, present in (1), are the same that in Ref. 21.

In order to investigate the influence of the nanostructure shape on the energy of the system we, firstly, find an expression for the Hamiltonian density $\mathcal{H}$. By definition

$$\mathcal{H} = \Pi\frac{\partial\vec{u}}{\partial t} - \mathcal{L}, \quad (3)$$

where

$$\Pi = \frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\vec{u}}{\partial t}\right)} = \rho\frac{\partial\vec{u}}{\partial t} \quad (4)$$

is the momentum density canonically conjugate to $\vec{u}$.

From the Lagrangian density (1) we obtain the following Hamiltonian density:

$$\mathcal{H} = \frac{1}{2\rho}\Pi^2 + \frac{1}{2}\rho\omega^2\vec{u}^2 + \alpha\vec{u}\cdot\nabla\phi - \frac{\varepsilon_\infty}{8\pi}|\nabla\phi|^2 - \frac{1}{2}\lambda_{ijkl}u_{ij}u_{kl}. \quad (5)$$

We must note that the momentum density canonically conjugate to ϕ is identically zero.

3. Hamiltonian operator

Taking into account (5) and working in the Schrödinger picture, the Hamiltonian operator describing the long-wavelength polar optical oscillations in the nanostructure is then given by

$$\hat{H} = \int \left(\frac{1}{2\rho}\hat{\Pi}^+\hat{\Pi} + \frac{1}{2}\rho\omega^2\hat{u}^+\hat{u} + \frac{\alpha}{2}\left[\hat{u}^+\nabla\hat{\phi} + \nabla\hat{\phi}^+\hat{u}\right] - \frac{\varepsilon_\infty}{8\pi}\nabla\hat{\phi}^+\nabla\hat{\phi} - \frac{1}{2}\lambda_{ijkl}\hat{u}_{ij}\hat{u}_{kl}\right) d^3r, \quad (6)$$

where $\hat{\Pi}$, $\hat{u}$, and $\hat{\phi}$ are the operators corresponding to the respective quantized fields and integration is extended to the whole nanostructure. The term corresponding to the coupling between electric field and mechanical vibrations has been symmetrized to ensure the Hamiltonian hermiticity.

The operators $\hat{\Pi}$, $\hat{u}$, and $\hat{\phi}$ may be written [21] in the form

$$\hat{\Pi} = -i\rho\sum_m [c_m\omega_m\vec{u}_m(\vec{r})\hat{b}_m - h.c], \quad (7)$$

$$\hat{u} = \sum_m [c_m\vec{u}_m(\vec{r})\hat{b}_m + h.c], \quad (8)$$

$$\hat{\phi} = \sum_m [c_m\phi_m(\vec{r})\hat{b}_m + h.c], \quad (9)$$

where $\vec{u}_m(\vec{r})$ and $\phi_m(\vec{r})$ are spatial solutions of the equations of motion generated by (1), corresponding to the m-th mode and ω_m its eigenfrequency. The operators $\hat{b}_m$ and $\hat{b}_m^+$ are the annihilation and creation operators respectively for a phonon in the m-th state, and c_m is the real constant:

$$c_m = \left(\frac{\hbar}{2\omega_m\Omega_0}\right)^{1/2}. \quad (10)$$

After tedious algebra we obtain

$$\hat{H} = \sum_m \mathcal{X}_m\left(\hat{b}_m^+\hat{b}_m + \frac{1}{2}\right) + \sum_m [\eta_m\hat{b}_m\hat{b}_m + h.c] + \hat{V}, \quad (11)$$

where $\mathcal{X}_m$ is the real quantity

$$\mathcal{X}_m = \hbar\omega_m + c_m^2\int\left(2\alpha\,\mathrm{Re}\,[\vec{u}_m\cdot\nabla\phi_m^*] - \frac{\varepsilon_\infty}{8\pi}|\nabla\phi_m|^2\right)d^3r - h_m, \quad (12)$$

with

$$h_m = c_m^2\sum_{(i,j)\epsilon S}\int\rho\left[2\beta_L^2\left|\frac{\partial u_{im}}{\partial x_i}\right|^2 + \beta_T^2\left|\frac{\partial u_{im}}{\partial x_j}\cdot\frac{\partial u_{jm}}{\partial x_i}\right|^2 + 2(\beta_L^2 - 2\beta_T^2)\mathrm{Re}\left(\frac{\partial u_{im}}{\partial x_i}\cdot\frac{\partial u_{jm}^*}{\partial x_j}\right)\right]d^3r. \quad (13)$$

Moreover, η_m is, in general, a complex quantity given by

$$\eta_m = c_m^2\int\left[\frac{\alpha}{2}(\vec{u}_m.\nabla\phi_m + \nabla\phi_m.\vec{u}_m) - \frac{\varepsilon_\infty}{8\pi}(\nabla\phi_m)^2\right]d^3r - g_m \quad (14)$$

with

$$g_m = \frac{c_m^2}{2}\sum_{(i,j)\epsilon S}\int\rho\left[2\beta_L^2\left(\frac{\partial u_{im}}{\partial x_i}\right)^2 + \beta_T^2\left(\frac{\partial u_{im}}{\partial x_j} + \frac{\partial u_{jm}}{\partial x_i}\right)^2 + 2(\beta_L^2 - 2\beta_T^2)\left(\frac{\partial u_{im}}{\partial x_i}\cdot\frac{\partial u_{jm}}{\partial x_j}\right)\right]d^3r. \quad (15)$$

In Eqs. (13) and (14) the indexes i, j indicate the component of the vector $\vec{u}_m(\vec{r})$ and m labels the mode. The summations over (i,j) run through the set of combinations $S = \{(1,2),(2,3),(3,1)\}$. Since we consider an isotropic medium, to obtain (13) and (14) we taken all non-zero components of the tensor λ_{ijkl} given by

$$\lambda_{iiii} = \rho\beta_L^2, \qquad \lambda_{iijj} = \rho(\beta_L^2 - 2\beta_L^2),$$
$$\lambda_{ijji} = \lambda_{ijij} = \rho\beta_T^2, \qquad (i,j = 1,2,3/i \neq j).$$

For more details see Refs. 21, 22 and 24.

In Eq. (11), the operator $\hat{V}$ describes the coupling between different modes. It gives rise to a small broadening of the energy levels, so it may be treated as a perturbation. However in this work, as a preliminary study, we neglect the coupling between different modes, that is, we assume that the lifetime of the elementary excitations is reasonably long, so that we dial with a simpler Hamiltonian

$$\hat{H}^{(o)} = \sum_m \mathcal{X}_m\left(\hat{b}_m^+\hat{b}_m + \frac{1}{2}\right) + \sum_m [\eta_m\hat{b}_m\hat{b}_m + h.c.]. \quad (16)$$

4. Energy spectrum

Once the Hamiltonian (16) is not diagonal in the phonon numbers, we will find the eigenvalues of (16) by diagonalizing the Hamiltonian using a linear transformation of the Bose-operators. Such a linear transformation is carried out by changing to new Bose-operators $\hat{A}_m$ through the equation

$$\hat{b}_m = \frac{|\kappa_m|}{\kappa_m}(\alpha_m \hat{A}_m + \beta_m \hat{A}_m^+), \tag{17}$$

where $\kappa_m^2 = \eta_m$ and α_m, β_m are real quantities satisfying

$$\alpha_m^2 + \beta_m^2 = \frac{\mathcal{X}_m}{\sqrt{\mathcal{X}_m^2 - 4|\eta_m|^2}} \tag{18}$$

and

$$\alpha_m \times \beta_m = \frac{-|\eta_m|}{\sqrt{\mathcal{X}_m^2 - 4|\eta_m|^2}}. \tag{19}$$

In terms of the new operators the Hamiltonian (16) results diagonal in the eigenvalues of the operators $\hat{N}_m = \hat{A}_m^+ \hat{A}_m$ and, it can be written as follows:

$$\hat{H} = \sum_m \hbar\xi_m(\hat{A}_m^+ \hat{A}_m + 1/2), \tag{20}$$

where

$$\xi_m = \frac{\sqrt{\mathcal{X}_m^2 - 4|\eta_m|^2}}{\hbar}. \tag{21}$$

We must note that η_m, $\mathcal{X}_m$ must satisfy the condition $2|\eta_m| < \mathcal{X}_m$ for the validity of our transformations, once we considered α_m, β_m as real quantities. It follows from (12), (14) that such a condition may be satisfied, if the oscillations are sufficiently small.

We must observe that, in the limit, when we ignore both the coupled electric field and the internal stress of the medium, Eq. (21) becomes $\xi_m = \omega_m$ as could be desired.

It follows from Eq. (20) that the states of the system described by the Lagrangian density (1) correspond to elementary excitations with energies $\hbar\xi_m$. It results remarkable, however, that because of the inclusion of the internal stress of the medium, the electric field and its coupling with the displacement, the energy of the long-wavelength polar optical phonons in SNS's depends not only on the frequencies ω_m, but also in a more complicated way on the nanostructure geometry.

5. Conclusions

In summary, we have derived, using a phenomenological treatment proposed in previous works, an approximated expression for the energy of elementary excitations in semiconductor nanostructures.

One must stress that the study of energy spectrum of optical vibrational quantum excitations in quantum wells, quantum well wires, superlattices and semiconducting heterostructures in general, as well as several thermodynamic properties such as heat capacity, may be readily obtained as straightforward applications [25] of the above approach on the physical properties of heterostructures.

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