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The polaron self-energy due to phonon confinement in quantum boxes and wires

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Abstract. The polaron self-energy due to phonon confinement in a quantum box or wire has been calculated as a function of the size of the quantum boxes or wires by the perturbative method using the framework of the effective mass approximation. It is found that the effects of phonon confinement are dominant in small boxes and wires. The results also show that it is a function of both width and thickness of the wire rather than simply the cross-sectional area.

1. Introduction

In recent years, with the advances in microfabrication technology such as molecular beam epitaxy (MBE), lithographic and etching techniques, ultrasmall semiconductor quantum wires [1–3] and quantum dots [4–8] have been successfully fabricated. A great deal of interest has been shown in the study of these structures because of their potential device applications and their success in uncovering new phenomena. As a consequence, understanding the electronic properties in such structures is of particular importance.

The exciton binding energies associated with the effects of the electron (hole)–optical–phonon interaction in quantum wires have been evaluated previously by Degani and Hipolito [9]. However, for the phonon system they have used the bulk-phonon approximation instead of the confined phonon. Indeed, phonon confinement has been shown by experiment [10].

The polaronic states may be affected by changes in the Frohlich Hamiltonian caused by phonon confinement. In a recent paper, Stroscio [11] has derived the one-dimensional Frohlich Hamiltonian describing the interaction of an electron and LO-phonon modes characterized by a travelling wave in the z-direction and standing waves in the x-direction and y-direction in a rectangular quantum-well wire. Size effects on the total scattering rates for the confined phonon scattering of one-dimensional electron gas have been calculated. More recently, several authors have reported calculations of the binding energy of impurity, excitaton and biexciton in quantum boxes [12–14]. However, they have not taken into account the interaction of the electron with the LO phonons. Brus

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[12] has calculated the energy levels of small semiconductor crystalline spheres under the effective-mass approximation, with which the dielectric polarization is partly considered.

Xia [15] has investigated the electronic structure of quantum dots and shown that the dielectric polarization of the small sphere lowers the binding energies, especially for a small radius. Pan *et al* [16] also calculated the energy of the charge carrier in a spherical semiconductor crystallite including the interaction of the charged carrier with phonons.

To date there is no published report on the interaction Hamiltonian of an electron with LO phonons in a quantum box. In this paper we shall derive the interaction Hamiltonian in a quantum box and use this Hamiltonian and the Hamiltonian derived by Stroscio to calculate the polaron self-energy due to phonon confinement in a quantum box and wire. Similar studies have been performed for a free polaron, impurity states and exciton levels in a polar crystal slab by one of the authors (S W Gu) and his co-writers [17–19].

In section 2 we derive the interaction Hamiltonian of an electron with LO phonons in a quantum box. Section 3 gives the calculation method in both quantum box and quantum wire. In section 4, the details of the numerical calculations are shown and the results are discussed. A brief conclusion is given in the last section.

2. The interaction Hamiltonian between an electron and LO phonons in a quantum box

The interaction Hamiltonian of an electron with the phonon modes in an ionic crystal slab has been derived by Licari and Evrard [20]. The resulting expression includes both the bulklike sinusoidal modes and the localized surface modes. The bulklike modes are equivalent to the bulk LO-phonon modes in three dimensions in the limit of an infinitely thick slab. In a similar way, Stroscio [11] has also derived the Frohlich Hamiltonian describing the interaction between LO-phonon modes of a rectangular quantum wire and charge carriers of a one-dimensional electron gas, and then used this Hamiltonian to calculate the total scattering rate.

To derive the Frohlich Hamiltonian describing the interaction of an electron and LO phonons in a zero-dimensional semiconductor material, the three-dimensional Frohlich Hamiltonian $H_i^{(3D)}$ must satisfy the boundary conditions governing the way in whch the LO-phonon potential vanishes in the x, y and z directions. $H_i^{(3D)}$ can be written

$$H_i^{(3D)} = \sum_K V_K \, e^{-iKr}(a_K + a_{-K}^{+}) \tag{1}$$

where K is a three-dimensional wavevector defined by

$$K = (k, k_z) = (k_x, k_y, k_z)$$

and

$$V_K = [2\pi e^2 \hbar \omega_{LO}(\varepsilon_0 - \varepsilon_\infty)/\varepsilon_0 \varepsilon_\infty V K^2]^{1/2} \tag{2}$$

where ω_{LO} is the frequency of the phonon, V is the crystal volume, ε_∞ is the high-frequency dielectric constant, and ε_0 is the low-frequency dielectric constant. If we divide the sum over K into a sum over k and a sum over $k_z > 0$, $H_i^{(3D)}$ becomes

$$H_i^{(3D)} = \sum_k \sum_{k_z>0} V_K \, e^{-ik\rho}[e^{-ik_z z}(a_{k,-k_z} + a^+_{-k,-k_z}) + e^{ik_z z}(a_{k,-k_z} + a^+_{-k,k_z})]. \tag{3}$$

To derive the Frohlich Hamiltonian for a phonon confined in three dimensions, we first define

$$\begin{cases} a_+(k) = [a_{k,k_z} + a_{k,-k_z}]/\sqrt{2} & (4a) \\ a_-(k) = -i[a_{k,k_z} + a_{k,-k_z}]/\sqrt{2} & (4b) \end{cases}$$

where the operators $a^\pm_+(-k)$ and $a^\pm_-(-k)$ follow by the definition of the adjoint.

Secondly, by defining

$$A_+(k_x)_\pm = [a_\pm(k_x, k_y) + a_\pm(k_x, -k_y)]/\sqrt{2} \tag{5a}$$

$$A_-(k_x)_\pm = -i[a_\pm(k_x, k_y) - a_\pm(k_x, -k_y)]/\sqrt{2}. \tag{5b}$$

Finally, by defining

$$\begin{cases} B_\pm(+)_\pm = [A_\pm(k_x)_\pm + A_\pm(-k_x)_\pm]/\sqrt{2} & (6a) \\ B_\pm(-)_\pm = -i[A_\pm(k_x)_\pm - A_\pm(-k_x)_\pm]/\sqrt{2} & (6b) \end{cases}$$

and taking $k_x = \pm m_1\pi/L_1$, $k_y = \pm m_2\pi/L_2$ and $k_z = \pm m_3\pi/L_3$ to ensure that box modes vanish at $x = \pm L_1/2$, $y = \pm L_2/2$ and $z = \pm L_3/2$ results in $H_i^{(OD)}$ which describes the interaction of an electron and LO-phonon modes characterized by standing waves in all three directions. Since its expression is similar to the case of the rectangular quantum wire derived by Stroscio [11], we neglect it here.

In the following we shall use this Hamiltonian and the Hamiltonian derived by Stroscio to calculate the electron self-energy in a quantum box and wire by the perturbative approach.

3. Theory

For the calculations described here, the boxes are assumed to be made of polar crystals, and are surrounded by a vacuum. To simplify the calculation we consider that the effective mass approximation is valid, which has been used in [12] and [15]. We also assume that the electrons are confined in infinitely deep potential wells in all three directions. In addition, mirror charge effects can be significant if there is a large dielectric discontinuity between the quantum box and the surrounding medium [12]. This is not the case for microfabricated boxes made, for example, with GaAs wells and AlGaAs barriers, therefore we ignore such effects here. We shall investigate such effects in the next paper.

The total Hamiltonian reads

$$H = H_e + H_{ph} + H_{e\text{-}ph}. \tag{7}$$

The first term H_e is the Hamiltonian of the electron in the infinite well potential and is given by

$$H_e = -(\hbar^2/2m^*)(\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2) \quad |x| \leqslant L_1/2 \quad |y| \leqslant L_2/2 \quad |z| \leqslant L_3/2. \tag{8}$$

The second term is the LO phonon operator,

$$H_{ph} = \sum_{m_1,p_1} \sum_{m_2,p_2} \sum_{m_3,p_3} \hbar\omega_{LO} B^+_{p_1,p_2,p_3}(m_1, m_2, m_3)\, B_{p_1,p_2,p_3}(m_1, m_2, m_3) \tag{9}$$

where $B^+_{p_1,p_2,p_3}(m_1, m_2, m_3)(B_{p_1,p_2,p_3}(m_1, m_2, m_3))$ is the creation (annihilation) operator for the LO phonon of frequency ω_{LO}. m_1, m_2 and m_3 are the x, y and z components of the total wavevector K. When m_1, m_2 and m_3 are odd or even, and p_1, p_2 and p_3 are positive (+) or negative (−).

It should be noted that the wavevector K of the LO-phonon is limited by the Brillouin zone boundary condition. That is, $m_1\pi/L_1 \leqslant \pi/2a$, $m_2\pi/L_2 \leqslant \pi/2a$, $m_3\pi/L_3 \leqslant \pi/2a$ (a is the lattice constant). From these inequalities, we can obtain: $1 \leqslant m_1 \leqslant N_1/2$ ($L_1 = N_1 a$), $1 \leqslant m_2 \leqslant N_2/2$ ($L_2 = N_2 a$), $1 \leqslant m_3 \leqslant N_3/2$ ($L_3 = N_3 a$).

The last term in (7) is the Hamiltonian of an electron interacting with the confined LO-phonons and is given by $H_i^{(OD)}$.

We separate the total Hamiltonian into two parts:

$$H = H_e + H_{ph} + H_{e\text{-}LO} = H_0 + H_{e\text{-}LO} \tag{10}$$

where

$$H_0 = -(\hbar^2/2m^*)(\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2) + \sum_{m_1,p_1} \sum_{m_2,p_2} \sum_{m_3,p_3} \hbar\omega_{LO} B^+_{p_1,p_2,p_3}(m_1,m_2,m_3) B_{p_1,p_2,p_3}(m_1,m_2,m_3). \tag{11}$$

Since $H_{e\text{-}LO}$ is small for the case of weak coupling, we can use the perturbative method.

In the low temperature limit, few phonons are excited. As a result, we assume that no real phonon exists in the phonon ground state and take $|0\rangle$ as the wavefunction for the phonon system, which must satisfy

$$B_{p_1,p_2,p_3}(m_1, m_2, m_3)|0\rangle = 0. \tag{12}$$

Using the perturbative method, the second order correction of the energy can be obtained. Since the expression is too complicated, we only give the numerical results.

4. Results and discussion

In this section we choose GaAs as an example to present the numerical results. In the calculations we have used the following parameters for GaAs: $a = 5.654$ Å^{-1}, $k_{LO} = 0.02516$ Å^{-1}, $\alpha = 0.0681$ and $\hbar\omega_{LO} = 36.70$ meV.

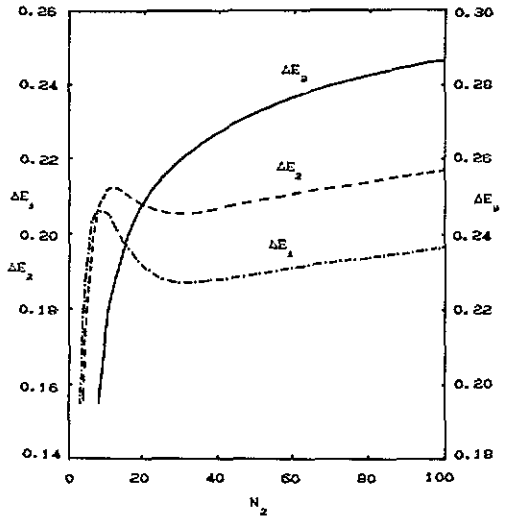

Figure 1. The electron self-energy of GaAs quantum well wires in units of $-\alpha\hbar\omega_{LO}$ as a function of the size of the wires. ΔE_1, $N_1 = 8$ (the chain curve); ΔE_2, $N_1 = 10$ (the broken curve); ΔE_3, $N_1 = 20$ (the full curve).

Figure 1 shows the electron self-energies due to the interaction of an electron with the confined LO-phonon as a function of the length of one side (N_2) of the wire for several values of the length of the other side (N_1). It is observed that as N_1 has small values ($N_1 \leqslant 12$), the self-energies have a peak at the beginning, and then increase slowly to the limit of the two-dimensional quantum well as N_2 approaches infinity. When N_1 is equal to N_2, the self-energy rises to the maximum of the peak. The smaller the size of the wire, the sharper the peak. As N_1 increases gradually, the peak moves to the right of the curve. When N_1 is larger than 12 layers, the peak disappears. In these cases, the features of the electron self-energies are similar to those in the two-dimensional wells. That is, the self-energies increase monotonically and slowly approach the two-dimensional limit value as N_2 is large enough. The reason for the appearance of a peak is that when the sizes of the wire are very small, the phonon is strongly confined in the quantum well wire. Upon enhancing the sizes of the wire, the effects of the phonon confinement are gradually weakened, the peak disappears, and the curve shows the behaviour of monotonical enhancement. As a result, for very small wires, we must take into account the effects of phonon confinement.

As we can see from the figures, the electron self-energies are related to the sizes of the wire rather than to the cross-sectional area of the wire. This result is different from the result obtained by Degani and Hipolito [9]. For example, $N_1 = 4$, $N_2 = 30$, $E = -0.32$ meV; $N_1 = 6, N_2 = 20, E = -0.42$ meV; $N_1 = 10, N_2 = 12, E = -0.53$ meV. We can also see that the absolute values of the electron self-energies are less than those in comparable two-dimensional quantum wells. We also note that the slow rise to the two-dimensional limit value after $N_2 = 100$ is somewhat strange, but this may simply be assigned to the neglect of the self-energy contribution of the interaction with the surface phonon.

Figure 2 shows the electron self-energies due to the interaction of electrons with the LO phonons as a function of the length of the cubic quantum boxes ($N_1 = N_2 = N_3$). It is observed that for small quantum cubes, the self-energies are enhanced with a decrease in the size of the quantum cubes. Figure 3 presents the electron self-energies as a function of the length of one side (N_3) of the box for several values of the length of the other two

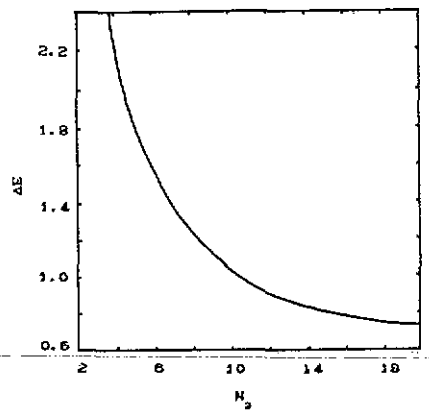

Figure 2. The electron self-energy of GaAs quantum cubes in units of $-\alpha\hbar\omega_{LO}$ as a function of the size of the cubes ($N_1 = N_2 = N_3$).

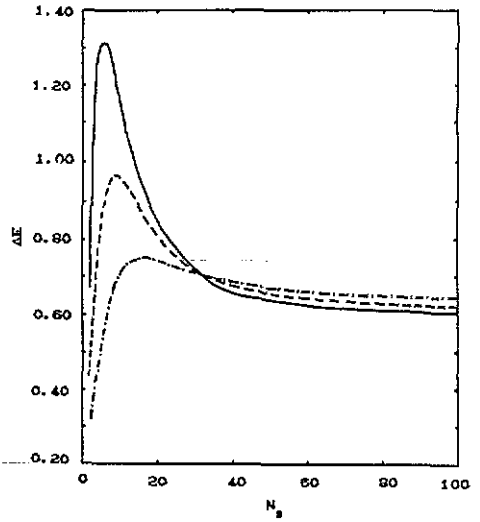

Figure 3. The electron self-energy of GaAs quantum boxes in units $-\alpha\hbar\omega_{LO}$ as a function of the size N_3 for several values of N_1 and N_2. $N_1 = N_2 = 8$ (the full curve); $N_1 = N_2 = 12$ (the chain curve); $N_1 = N_2 = 20$ (the broken curve).

sides ($N_1 = N_2$). From the figures we can see that the self-energy increases rapidly to a maximum and then decreases slowly to the limit of the wire case as N_3 approaches infinity while remaining fixed in the other two directions (N_1 and N_2).

For smaller N_1 and N_2, the peak is sharper. The reason for the appearance of a peak is that as the size of the box is small, the phonon is strongly confined in the quantum box. With an increase of the size of the box, the effect of phonon confinement is gradually weakened and the peak is smoothed. This result is just like the wire case. As $N_1 = N_2 = 40$, the peak still exists. Therefore, for small boxes the effects of phonon confinement must be taken into account. From the calculations we notice that the self-energy still has the features of those in $N_1 = N_2 = 20$ even though $N_1 = N_2 = 6$. This may imply that as $N_1 = N_2 = 6$, the approximation we used here is still available. In addition, as we can see from the figures the maximum of the self-energies at small N_1 and N_2 is larger than at large N_1 and N_2 with increasing N_3.

5. Conclusions

The electron self-energies due to the interaction of an electron with the LO-phonons that incorporate the effects of phonon confinement in a rectangular quantum-well wire and a quantum box have been calculated as a function of the sizes of the quantum boxes and wires by the perturbative method. In the calculations, we have used the continuum approximation in which the lattice is treated as a polarizable continuum and the effective-mass approximation is used for the electron. As regards the corrections to the continuum approximation, Lepine and Frongillo [21] have recently investigated the effects of the corrections to the continuum approximation in the Frohlich Hamiltonian and have

shown that for the polar crystals, the corrections to the continuum approximation are rather small, the largest one being of the order of 3% for the case of weak-coupling polar crystals. The results show that the effects of phonon confinement are dominant in small boxes and wires, and must be taken into account. We also find that the self-energies are related to the sizes of the cross-section rather than to the cross-sectional area of the wire.

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