# Influence of Phonon Confinement on the Optically-detected Electrophonon Resonance Linewidth in Rectangular Quantum Wires

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We investigate the influence of phonon confinement on the optically-detected electrophonon resonance (ODEPR) effect and ODEPR linewidth in rectangular quantum wires (RQW). The ODEPR conditions as functions of the wire's size and the photon energy are also obtained. The splittings of ODEPR peaks caused by the confined phonon are discussed. The numerical result for a specific RQW shows that in the two cases of confined and bulk phonons, the linewidth decreases with increasing wire size and increases with increasing temperature. Furthermore, in the small range of the wire's size ( $L \leq 40$  nm), phonon confinement plays an important role and cannot be neglected in reaching the ODEPR linewidth.

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#### I. INTRODUCTION

The absorption linewidth (LW) is well known as a good tool for investigating the scattering mechanisms of carriers and, hence, can be used to probe electron-phonon scattering processes. To investigate the effects of various scattering processes, absorption LWs have been measured in various kind of semiconductors, such as quantum wells [1–6], quantum wires [7–10], and quantum dots [11–15]. These results show that the absorption LW has a weak dependence on temperature and has a strong dependence on system size. However, in those articles, the absorption LW was investigated based on the interaction of electrons and bulk phonons, but the absorption LW in rectangular quantum wires due to the confined-LOphonon-electron interaction is still open for study.

It is well known that the effects of confinement of phonons should be taken into account in order to obtain realistic estimates for electron-phonon scattering [16– 18]. Phonon confinement affects optically-detected electrophonon resonance (ODEPR) effect mainly through changes in the selection rules for transitions involving subband electrons and affects the ODEPR line width (ODEPRLW) through changes in the probability of electron-phonon scattering. The LW is defined by the profile of the curves describing the dependence of absorption power  $P(\omega)$  on the photon energy or frequency [19, 20]. Recently, our group has proposed a method, called the profile method, to computationally obtain the LW from graphs of  $P(\omega)$  [21] and used this method to determine cyclotron resonance linewidth in cylindrical quantum wires [22], and in GaAs/AlAs quantum wires [23].

In the present work we investigate the intersubband ODEPRLW in a rectangular quantum wire (RQW). We study the dependence of the ODEPRLW on the wire's size  $L_x$  ( $L_y$ ) and the temperature T. The result of the present work is fairly different from previous results because the phonon confinement is taken into account and because the results can be applied to optically detect the resonant peaks.

#### II. MODEL OF A RQW

We consider a quantum wire with a rectangular crosssection along the z axis and with finite x and y dimensions given by  $L_x$  and  $L_y$ , respectively. We assume that the confining potential well is an infinite square well. Both electrons and phonons are confined. They differ essentially in the way the boundary conditions are applied [24]. In this case, the electron wave function has the well known form

$$|\alpha\rangle \equiv |m, n, k_z\rangle = \frac{e^{ik_z z}}{\sqrt{L_z}} \frac{2}{\sqrt{L_x L_y}} \sin \frac{m\pi x}{L_x} \sin \frac{n\pi y}{L_y}, \quad (1)$$

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where  $L_z$  is the length of the quantum wire,  $0 \le x \le L_x$ and  $0 \le y \le L_y$ . The corresponding electron energy is

$$E_{\alpha}(k_z) \equiv E_{m,n}(k_z) = \frac{\hbar^2 k_z^2}{2m^*} + \frac{\pi^2 \hbar^2}{2m^*} \left(\frac{m^2}{L_x^2} + \frac{n^2}{L_y^2}\right)$$
$$= \frac{\hbar^2 k_z^2}{2m^*} + E_{m,n}, \qquad (2)$$

where  $k_z$  is the electron wave vector along the wire axis,  $m, n = 1, 2, 3, \ldots$  denote the quantum numbers and  $m^*$ is the electron effective mass.

In this paper, we use the model of confined phonons presented by Constantinou and Ridley [25], where the frequency of a mode labeled  $(\ell, j)$  is given by

$$\omega_q^2 = \omega_{LO}^2 - \beta^2 (q_z^2 + q_{\ell j}^2), \ q_{\ell j}^2 = \left(\frac{\ell \pi}{L_x}\right)^2 + \left(\frac{j\pi}{L_y}\right)^2, \ (3)$$

with  $\omega_{LO}$  being the zone-center LO-phonon frequency, and  $\beta$  the velocity parameter (  $\beta = 4.73 \times 10^3$  $ms^{-1}$  for GaAs). We have phonon along the wire's axis. For the calculation of the absorption power of an also assumed that  $q_{\ell i} \gg q_z$ , with  $q_z$  being the wave vector of a electromagnetic wave in a RQW, the following matrix elements are used [24]:

$$\begin{aligned} |\langle \alpha | e^{\pm i \vec{q} \cdot \vec{r}} | \alpha' \rangle|^2 &= |P_{m,n,m',n'}^{\ell,j}|^2 \delta_{k'_z,k_z \pm q_z}, \end{aligned} \tag{4} \\ P_{m,n,m',n'}^{\ell,j} &= \frac{4}{L_x L_y} \int_0^{L_x} dx \int_0^{L_y} dy \sin \frac{m \pi x}{L_x} \sin \frac{m' \pi x}{L_x} \sin \frac{n \pi y}{L_y} \sin \frac{n' \pi y}{L_y} \sin \frac{\ell \pi x}{L_x} \sin \frac{j \pi y}{L_y}. \end{aligned} \tag{5}$$

The lowest-orders of  $P_{m,n,m',n'}^{\ell,j}$  are calculated as  $P_{1,1,1,1}^{1,1} = (8/3\pi)^2$ ,  $P_{1,1,2,1}^{1,1} = P_{2,1,1,1}^{1,1} = (1/4)$ , and  $P_{1,1,3,1}^{1,1} = P_{3,1,1,1}^{1,1} = (1/25)(8/3\pi)^2$ .

### **III. ABSORPTION POWER IN A RQW**

When an electromagnetic wave characterized by a time-dependent electric field of amplitude  $E_0$  and angular frequency  $\omega$  is applied, the absorption power  $P(\omega)$ delivered to the system is given by  $P(\omega) = (E_0^2/2)$  $\operatorname{Re}\{\sigma_{ij}(\omega)\}\ [26,27].$  Here,  $\sigma_{ij}(\omega)$  is the *ij*-component of the optical conductivity tensor. If the general expression for the conductivity presented by Kang et al. [28] and Lee et al. [29] in a rectangular quantum wire is used, the absorption power is given, at the subband edge  $(k_z = 0)$ , by the following expression:

$$\operatorname{Re}\{\sigma_{xx}(\omega)\} = e^{2} \sum_{m,n} \sum_{m',n'} |(x)_{m,m'}| |(j_{x})_{m,m'}| \frac{(f_{m',n'} - f_{m,n})B(\omega)}{[\hbar\omega - (E_{m',n'} - E_{m,n})]^{2} + [B(\omega)]^{2}}.$$
(6)

Here, e is the charge of a conduction electron;  $E_{m,n}$ and  $E_{m',n'}$  are the energies of the electron in the initial  $\alpha \equiv |m, n, 0 >$  and the final state  $\beta \equiv |m', n', 0 >$ , respectively;  $f_{m,n}$  is the Fermi-Dirac distribution function of an electron with energy  $E_{m,n}$ ; and  $|(x)_{m,m'}|$  is the matrix element of the position operator, given by

$$|(x)_{m,m'}| = \frac{L_x}{\pi L_z} \delta_{n,n'} \begin{cases} \frac{1}{2\pi^2} \left[ \frac{(-1)^{m-m'} - 1}{(m-m')^2} - \frac{(-1)^{m+m'} - 1}{(m+m')^2} \right], & m \neq m' \\ \frac{1}{4}, & m = m'. \end{cases}$$
(7)

The matrix element  $|(j_x)_{m,m'}|$  of the current operator is

$$|(j_x)_{m,m'}| = \frac{e\hbar m}{L_z m^*} \begin{cases} \frac{(-1)^{m+m'}-1}{m+m'} + \frac{(-1)^{-m+m'}-1}{m'-m}, & m \neq m'\\ 0, & m = m'. \end{cases}$$
(8)

In Eq. (6),  $B(\omega)$  is the imaginary part of the damping function which was obtained in Refs. 28 and 29 as

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$$B(\omega) = \frac{\pi}{(f_{\beta} - f_{\alpha})} \sum_{\mu,q} |C_{\beta\mu}(q)|^{2} \Big\{ [(1 + N_{q})f_{\alpha}(1 - f_{\mu}) - N_{q}f_{\mu}(1 - f_{\alpha})] \delta(\hbar\omega - E_{\mu} + E_{\alpha} - \hbar\omega_{q}) \\ + [N_{q}f_{\alpha}(1 - f_{\mu}) - (1 + N_{q})f_{\mu}(1 - f_{\alpha})] \delta(\hbar\omega - E_{\mu} + E_{\alpha} + \hbar\omega_{q}) \Big\} + \pi \sum_{\mu,q} |C_{\alpha\mu}(q)|^{2} \\ \times \Big\{ [(1 + N_{q})f_{\mu}(1 - f_{\beta}) - N_{q}f_{\beta}(1 - f_{\mu})] \delta(\hbar\omega - E_{\beta} + E_{\mu} - \hbar\omega_{q}) \\ + [N_{q}f_{\mu}(1 - f_{\beta}) - (1 + N_{q})f_{\beta}(1 - f_{\mu})] \delta(\hbar\omega - E_{\beta} + E_{\mu} + \hbar\omega_{q}) \Big\}.$$
(9)

Here,  $\delta(\ldots)$  is Dirac's delta function;  $N_q$  is the Planck distribution function for a phonon in the state  $|q\rangle = |\ell, j, q_z\rangle$ ;  $C_{\beta\mu}(q)$  is the electron-phonon interaction matrix elements and depends on the scattering mechanism. In this model it is given by

$$C_{\beta\mu}(q) = C_{\ell,j}(q_z) P_{m',n',m'',n''}^{\ell,j} \delta_{k_z^\beta,k_z^\mu + q_z}$$
(10)

with  $|\mu\rangle \equiv |m^{"}, n^{"}, k_{z}^{\mu}\rangle$  being the intermediate states. In Eq. (10), the expression of the coupling factor  $|C_{\ell,j}(q_{z})|$  is given as [30,31]

$$|C_{\ell,j}(q_z)|^2 = \frac{C}{q_{\ell j}^2 + q_z^2},$$
  

$$C = \frac{2\pi e^2 \hbar \omega_{LO}}{\varepsilon_0 \Omega} \left(\frac{1}{\chi_{\infty}} - \frac{1}{\chi_0}\right),$$
(11)

where  $\varepsilon_0$  is the permittivity of free space,  $\chi_{\infty}$  and  $\chi_0$  are the high and the low frequency dielectric constants, and  $\Omega = L_x L_y L_z$  is the volume of the quantum wire.

To calculate  $\operatorname{Re}\{\sigma_{xx}(\omega)\}$  given in Eq. (6), we need to determine  $B(\omega)$  in Eq. (9). Converting summations into integrals as  $\sum_{q} \rightarrow \frac{L_z}{2\pi} \sum_{\ell,j} \int_{-\infty}^{+\infty} dq_z$  and  $\sum_{\mu} \rightarrow \frac{L_z}{2\pi} \sum_{m'',n''} \int_{-\infty}^{+\infty} dk_z^{\mu}$ , the power absorption in the systems for the transition between the two sublevels will be calculated at the band edge  $(k_z^{\alpha} = 0)$ . Note that the selection rule requires  $k_z^{\alpha} = k_z^{\beta}$  or a direct transition. After some mathematical manipulation, we have

$$B(\omega) = \frac{1}{(f_{m',n'} - f_{m,n})} \sum_{m'',n''} \sum_{\ell,j} \left\{ \frac{|I_{m'',n'',m',n''}^{\ell,j}|^2}{(Q_1^2 + q_{\ell,j}^2)Y^{(-)}(Q_1, q_{\ell,j})} [(1 + N_q)f_{m,n,0}(1 - f_{m'',n'',Q_1}) - (1 + N_q)f_{m'',n'',Q_1}(1 - f_{m,n,0})] \right. \\ \left. + \frac{|I_{m'',n'',m',n'}^{\ell,j}|^2}{(Q_1^2 + q_{\ell,j}^2)Y^{(+)}(Q_1, q_{\ell,j})} [N_q f_{m,n,0}(1 - f_{m'',n'',Q_1}) - (1 + N_q)f_{m'',n'',Q_1}(1 - f_{m,n,0})] \right. \\ \left. + \frac{|I_{m,n,m'',n''}^{\ell,j}|^2}{(Q_2^2 + q_{\ell,j}^2)Y^{(+)}(Q_2, q_{\ell,j})} [(1 + N_q)f_{m'',n'',Q_2}(1 - f_{m',n',0}) - N_q f_{m',n',0}(1 - f_{m'',n'',Q_2})] \right. \\ \left. + \frac{|I_{m,n,m'',n''}^{\ell,j}|^2}{(Q_2^2 + q_{\ell,j}^2)Y^{(-)}(Q_2, q_{\ell,j})} [N_q f_{m'',n'',Q_2}(1 - f_{m',n',0}) - (1 + N_q)f_{m',n',0}(1 - f_{m'',n'',Q_2})] \right\}.$$
(12)

Here,

$$Y^{\pm}(Q_{i},q_{\ell,j}) = \left| \frac{\hbar^{2}\beta^{2}}{(\omega_{0}^{2} - \beta^{2}(q_{\ell,j}^{2} + Q_{i}^{2}))^{1/2}} \pm \frac{\hbar^{2}}{m^{*}} \right|, \qquad Q_{i} = [a_{i} \pm (a_{i}^{2} - b_{i})^{1/2}]^{1/2},$$

$$a_{i} = \frac{2m^{*}}{\hbar^{2}}(\hbar\omega - \Delta E_{\mu\alpha} - m^{*}\beta^{2}), \qquad b_{i} = \frac{4m^{*2}}{\hbar^{4}}[(\hbar\omega - |\Delta E_{\mu i}|)^{2} - \hbar^{2}(\omega_{0}^{2} - \beta^{2}q_{\ell,j}^{2})],$$

$$f_{m'',n'',Q_{i}} = \{1 + \exp[(E_{m'',n'',Q_{i}} - E_{F})/(k_{B}T)]\}^{-1}, \qquad E_{m'',n'',Q_{i}} = \frac{\hbar^{2}Q_{i}^{2}}{2m^{*}} + E_{m'',n''}.$$

Inserting Eq. (12) into Eq. (6), we will obtain an explicit expression for  $\operatorname{Re}\{\sigma_{xx}(\omega)\}$ . That is, we have ob-

tained an expression for the absorption power in a rectan-

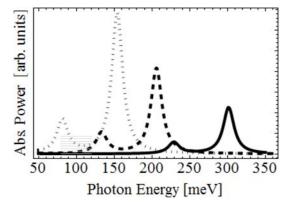


Fig. 1. Dependence of the AP on the photon energy for the different values of the wire's size. The solid, the dashed and the dotted curves correspond to L = 8 nm, L = 10 nm, and L = 12 nm, respectively. Here, T = 300 K.

gular quantum wire. We can see that these analytical results appear very involved. However, physical conclusions can be drawn from graphical representations and numerical results, obtained from adequate computational methods.

# IV. NUMERICAL RESULTS AND DISCUSSION

The expression of  $B(\omega)$  in Eq. (12) exhibits a resonant behavior due to the ODEPR condition

$$\hbar\omega \pm \Delta E_{m,n,m',n'} \pm \hbar\omega_q = 0, \qquad (13)$$

where  $\Delta E_{m,n,m',n'} = E_{m,n} - E_{m',n'}$ . Equation (13) is the ODEPR condition in a rectangular quantum wire. This result is the same as Lee's result for a quantum wire with a Woods-Saxon potential [32] and in a quantum well [33]. When the ODEPR conditions are satisfied, in the course of scattering events, electrons in the state  $|m,n\rangle$  can transition to another state  $|m',n'\rangle$  by absorbing a photon of energy  $\hbar\omega$  during the absorption and/or emission of a confined LO-phonon of energy  $\hbar \omega_{\ell i}$ . To clarify the obtained results, we numerically calculate the absorption power  $P(\omega)$  for a specific RQW made up of GaAs/AlAs. The absorption power is considered to be a function of the photon energy. The parameters used in our calculations are as follows [31, 34]:  $\varepsilon_0 = 12.5$ ,  $\chi_{\infty} = 10.9, \, \chi_0 = 13.1, \, m^* = 0.067 m_0 \, (m_0 \text{ being the})$ electron rest mass), and  $\hbar\omega_{LO} = 36.25$  meV. The dominant contribution to the sum over phonon modes in Eq. (5) is well known to be the mode with  $\ell = j = 1$ . The conclusion that follows will be calculated in the extreme quantum limit, where only the lowest subbands is occupied, *i.e.*, m = 1, n = 1, m' = 2, n' = 1.

In Fig. 1, the solid curve (L = 8 nm) corresponds to  $\Delta E_{2,1,1,1} = 265.08 \text{ meV}$  and to the energy of confined phonon  $\hbar \omega_{11} = 36.21 \text{ meV}$ . By using the computational

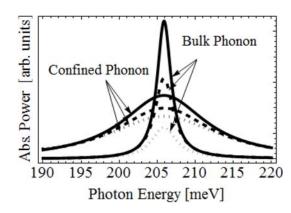


Fig. 2. Dependence of the AP on the photon energy at the ODEPR peaks for phonon absorption processes. The solid, the dashed and the dotted curves correspond to T = 100 K, T = 200 K, and T = 300 K, respectively. Here, L = 10 nm.

method, we easily determine that peaks 1 and 2 (of this curve) correspond to the values  $\hbar \omega^- = 228.87$  meV and  $\hbar\omega^+ = 301.29$  meV, respectively. These two peaks satisfy the ODEPR conditions  $\hbar\omega^{\mp} = \Delta E_{2,1,1,1} \mp \hbar\omega_{11}$ , or  $\hbar\omega^{\mp} = 265.08 \mp 36.21$  meV. They arise from the transitions of an electron from the energy level  $E_{1,1}$  to the energy level  $E_{2,1}$  by absorbing a photon  $\hbar\omega^-(\hbar\omega^+)$ and emitting (absorbing) a phonon  $\hbar\omega_{11}$ . The distance between these two peaks (in the unit of energy) is  $\Delta \hbar \omega = \hbar \omega^+ - \hbar \omega^- = 72.42$  meV; this value is twice as much as the confined phonon energy  $\hbar\omega_{11}$ . The cases of L = 10 nm (dashed curve) and L = 12 nm (dotted curve) can be understood similarly. However, in each curve, the distance between two resonant peaks, as well as the confined phonon energy  $\hbar\omega_{11}$ , is seen to decrease as L increases, but the distance between the two peaks is always twice as much as the phonon energy.

From Fig. 1, when the wire's size increases, the resonant peaks is seen to shift to the left (the small region of photon energy) because of the decreasing of  $\Delta E_{2,1,1,1}$  when the wire's size L increases; consequently, the photon energy that satisfies the ODEPR condition decreases. Moreover, the second peak of each curve is always higher than the first one. This means that the phonon absorption processes are more dominant than the emission processes. In the following, we will use the second peak of each curve to consider the influence of the phonon confinement on the LWs of the ODEPR peaks. To do this, we plot the dependence of AP on the photon energy for both models: the bulk-phonon (3D) and the confined-phonon models.

In Fig. 2, we can see that all the peaks in the case of bulk phonons are located at  $\hbar\omega_{\text{bulk}} = 205.90 \text{ meV}$  while the peaks in the case of confined phonon absorption are at  $\hbar\omega_{\text{conf}} = 205.89 \text{ meV}$ . The difference between these two values is seen not to be considerable and can be neglected. Thus, the phonon confinement does not have an effect on the peak location of the ODEPR. The appearances of resonant peaks at the same value of the photon

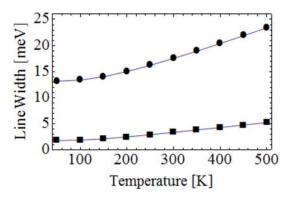


Fig. 3. (Color online) LW as a function of the temperature for different models of phonon. The closed squares and the closed circles correspond to the bulk-phonon model and the confined-phonon model, respectively. Here, L = 10 nm.

energy also show that the ODEPR does not depend on the temperature. However, the influence of the phonon confinement is much more considerable when we consider the LW. In Fig. 2, the LWs in the case of confined phonons are easily seen to be larger than they are in the case of bulk phonons. However, a detailed evaluation can be performed by using the profile method [21]. This is a method of determining the LW based on graphs of AP versus the photon energy with the help of a computational program. It was suggested by our group and has been applied successfully in some of our recent works.

In order to find the dependence of LW on temperature, we first plot the graph showing the dependence of the AP on the photon energy for different values of temperature. Then, we use a command of Mathematica software to find the two values of the photon energy,  $\hbar\omega_1$  and  $\hbar\omega_1$ , corresponding to a half-maximum of the absorption power. One pair of  $(T, \hbar\Delta\omega = \hbar\omega_2 - \hbar\omega_1)$  represents one point on the curve of the graph. Joining these points, we obtain the rule showing the dependence of LW on temperature. The dependence of LW on the temperature is shown in Fig. 3. From Fig. 3 we can see that the LW increases with increasing temperature in both models of phonon (the bulk-phonon and confined-phonon models). Physically, this is reasonable because the possibility of electron-phonon scattering rises as the temperature increases. The LWs for confined phonons are also seen to be larger than they are for bulk phonons. This means that phonon confinement gives raise to the possibility of electron-phonon scattering.

In Fig. 4, the AP is plotted versus the photon energy for the two above-mentioned models of phonons at the different values of the wire's size. From the figure, we can see that the resonant peaks shift to smaller photon energy when the wire's size increases. The appearance of these peaks can be explained by using the ODEPR condition, as shown above in Fig. 1. For each value of the photon energy at the resonance, the LW for confined phonons is always larger than it is for the corresponding bulk phonons.

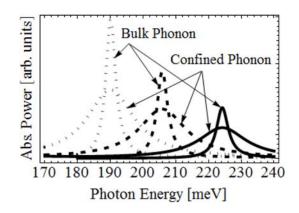


Fig. 4. Dependence of the AP on the photon energy at the ODEPR peaks for phonon absorption processes. The solid, the dashed and the dotted curves correspond to L = 9.5 nm, L = 10.0 nm, and L = 10.5 nm, respectively. Here, T = 300 K.

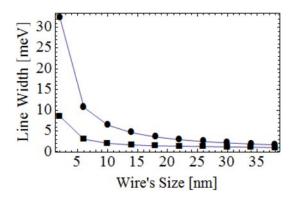


Fig. 5. (Color online) LW as a function of the wire's size for different models of phonon. The closed squares and the closed circles correspond to the bulk-phonon model and the confined-phonon model, respectively. Here, T = 300 K.

We found the dependence of the LW on the wire's size in the same way as we found the dependence of LW on the temperature. The dependence of the LW on the wire's size is shown in Fig. 5. From Fig. 5, we can see that the LW decreases with increasing of the wire size for both models of the phonon. The result is consistent with that shown in some previous works [2, 8, 9]. This can be explained physically by a decrease in the possibility of electron - phonon scattering when the wire's size increases. Furthermore, the LW for the confined-phonon case varies faster and has a larger value than it does for the bulkphonon case, and the smaller the wire's size is, the more pronounced the difference is. Thus, as the wire's size decreases, the phonon confinement becomes more important and cannot be neglected. For wires with sizes larger than 40 nm, the influence of phonon confinement on the LW is very small and can be ignored.

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# V. CONCLUSION

In the present paper, we calculated analytical expressions for the conductivity tensor and the absorption power in a RQW due to the confined electron - confined LO phonon interaction. From the graphs of the absorption power  $P(\omega)$ , we obtained the LW as profiles of curves. Computational results show that in the cases of both bulk and confined phonons, the LW increases with increasing temperature and decreases with increasing wire size. In addition, the value of the LW in the case of confined phonons is greater than and asymptotic to that in the case of bulk phonons when L increases. However, for wires with sizes larger than 40 nm, the influence of the phonon confinement on the LW is very small and can be ignored. This result is the same as that obtained in a two-dimensional system, which is verified by theory and experiments.

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