

Confined optical phonon effects on the band gap renormalisation in quantum wire structures

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Abstract

We consider the different approximations for the bandgap renormalisation (BGR) within the random phase approximation (RPA), the quasi-static limit and the plasmon-pole approximation, and compare with the full result. We then include bulk optical phonons and also the phonon confinement using the phonons from the dielectric continuum (DC) model. We show that the results are very similar except at low densities where the quasi-static results overestimate the renormalisation. © 1999 Elsevier Science B.V. All rights reserved.

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Quantum wire structures have been produced as laser devices due to the expectation of a low threshold current and temperature dependence. The emission wavelength depends on the bandgap of the wire material which will be renormalised by the electrons and holes present and their coupling with the optical phonons in the system. Recent experiments [1,9] have measured this bandgap renormalisation (BGR) for high electron and hole densities produced by photo-excitation and the results have been successfully modelled using a quasi-static approximation [2,10]. Our aim in this paper is to compare the various approximations of the BGR within the random phase approximation (RPA) and include the effect of bulk optical phonons and the confined phonons from the dielectric continuum (DC) model.

The self energy of electrons ($j = 1$) or holes ($j = 2$) at zero temperature is given by

$$\Sigma^j(k, \omega) = i \int \frac{dq}{2\pi} \int \frac{d\omega'}{2\pi} \frac{V(q)}{\varepsilon(q, \omega')} G_0^j(k+q, \omega+\omega'), \quad (1)$$

where the BGR is the sum of the self energy of the electrons and holes when $k = 0$ and $\omega = 0$. We assume that the density n of the electrons and holes is the same, as would be the case in photo-excitation. Eq. (1) may be decomposed into, respectively, the exchange, line and pole terms [3]

$$\Sigma_{\text{ex}}^j(0, 0) = -2 \int_0^{k_c} \frac{dq}{2\pi} V(q), \quad (2a)$$

$$\Sigma_{\text{line}}^j(0, 0) = 4 \int_0^\infty \frac{dq}{2\pi} \int_0^\infty \frac{d\omega}{2\pi} V(q) \left[\frac{1}{\varepsilon(q, \omega)} - 1 \right] \times \frac{E_q^j}{(E_q^j)^2 + (\hbar\omega)^2}, \quad (2b)$$

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$$\Sigma_{\text{pole}}^j(0, 0) = -2 \int_0^{k_f} \frac{dq}{2\pi} V(q) \left[\frac{1}{\varepsilon(q, E_q^j/\hbar)} - 1 \right], \quad (2c)$$

only the real parts are required and $E_q^j = \hbar^2 q^2 / 2m_j^*$. We use the dielectric function given by the RPA and the Lindhard function $\chi_j(q, \omega)$ [5],

$$\varepsilon(q, \omega) = \left[1 + \frac{V_{\text{ph}}(q, \omega)}{V(q)} \right]^{-1} - V(q) [\chi_1(q, \omega) + \chi_2(q, \omega)], \quad (3)$$

where $V(q)$ is the Coulomb potential, $V_{\text{ph}}(q, \omega)$ is the phonon potential and we assume a cylindrical quantum wire with a radius R . The general form for this phonon potential is [4] $V_{\text{ph}}(q, \omega) = \sum_{\text{all modes}} |M(q)|^2 D(q, \omega, \omega_q)$, where $|M(q)|^2$ is the squared matrix element of the interaction between the carriers and phonons concerned, ω_q is the phonon frequency and $D(q, \omega, \omega_q)$ is the phonon propagator given by [4] $D(q, \omega, \omega_q) = 2\omega_q / \hbar(\omega^2 - \omega_q^2)$. To ignore the phonon contribution $V_{\text{ph}}(q, \omega)$ is set to zero. For bulk phonons the matrix element is given by [4] $|M_b(q)|^2 = V(q)\hbar\omega \times (1 - \varepsilon_\infty/\varepsilon_s)/2$. For the DC phonons we have the sum of the confined and interface phonon terms. For the matrix elements and phonon potentials of the DC phonons the reader is directed to Refs. [5,6].

If the phonons are included when calculating the BGR, we should subtract the self energy due solely to the phonons, since these are always present and any experiment will not detect their separate influence. Hence, we must subtract the self energy given by perturbation theory,

$$\Delta E = - \sum_{\text{all modes}} \sum_j \frac{|M(q)|^2}{\hbar\omega_q + E_q^j}. \quad (4)$$

This reduction is included in all of the graphs shown where phonons are included.

We may approximate the Lindhard function in Eq. (3) with the plasmon-pole approximation where we satisfy the f-sum rule and the static limit [4] and assume that all of the weight of the dielectric function is at a series of poles. This gives the approximation to Eq. (3),

$$\varepsilon(q, \omega) \approx \left[1 + \frac{V_{\text{ph}}(q, \omega)}{V(q)} \right]^{-1} - \frac{\omega_1^2}{\omega^2 - \omega_{q1}^2} - \frac{\omega_2^2}{\omega^2 - \omega_{q2}^2}. \quad (5)$$

Here $\omega_j^2 = V(q)nq^2/m_j^*$ and $\omega_{qj}^2 = -nq^2/m_j^*\chi_j(q, 0)$. Das Sarma et al. [7] have shown that the plasmon-pole approximation describes the quasi-particle properties of one-dimensional structures quite well.

Using Eq. (5) we may rewrite the terms in Eqs. (2a)–(2c) as a series of pole-like terms and reduce the frequency integration in the line term analytically to leave one integration over q and also simplify the pole integration. Without the phonons there are two poles while including the bulk phonons produces three poles in the dielectric function.

Finally, we may make the most extreme approximation by replacing the dielectric function by the static dielectric function. This should be valid for high densities when k_f is large. The quasi-static approximation for the BGR is

$$\Sigma(0, 0) = -2 \int_0^{k_f} \frac{dq}{2\pi} \frac{V(q)}{\varepsilon(q, 0)} - 2 \int_0^\infty \frac{dq}{2\pi} V(q) \times \left[\frac{1}{\varepsilon(q, 0)} - 1 \right], \quad (6)$$

normally written as the screened exchange and Coulomb-hole terms.

Fig. 1 shows the full result and the plasmon-pole and quasi-static approximations with and without bulk GaAs phonons for a GaAs quantum wire. The plasmon-pole approximation appears to be accurate, although moving closer to the quasi-static result, for the range of densities shown, however, computationally this can be complicated by the integration over the poles. It can also be seen that the quasi-static result overestimates the BGR for small densities but, as expected, is accurate for large densities. These large densities are where the experiments, up until now, have been performed [1]. The inclusion of the bulk phonons decreases the discrepancy of the quasi-static result at low densities (this is due to the subtraction of the self energy due solely to the phonons without an increase in the coupled mode self energy) and also produces a larger BGR at high densities where ε_∞ is the relevant dielectric constant not ε_s .

Fig. 2 shows the effect of the phonon confinement with quantum wire radius. For small radii the BGR becomes infinite but should tend towards the result with bulk AlAs phonons. For larger radii the result tends towards the curve including bulk GaAs

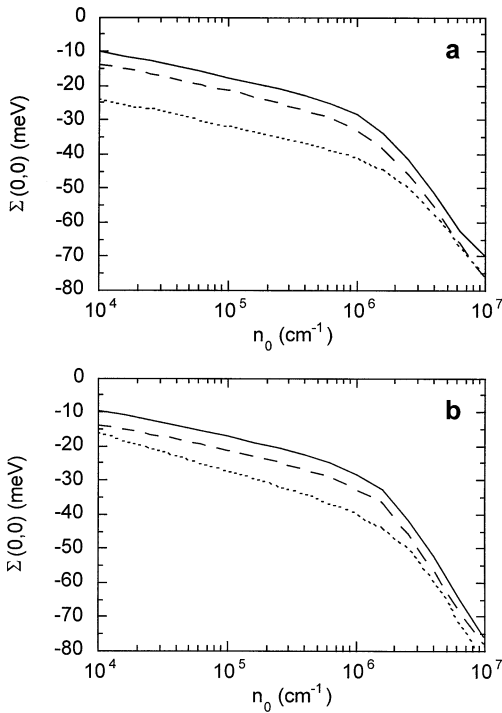


Fig. 1. The bandgap renormalisation against density for a GaAs quantum wire of radius $R = 50 \text{ \AA}$ (a) without and (b) including bulk GaAs phonons for the full result (solid), the plasmon-pole approximation (dashed) and the quasi-static limit (dotted).

phonons. This is expected from the sum-rule governing the DC model [8]. We can see that the inclusion of optical phonon confinement is not important but does produce a result between the BGR using the bulk phonons of the two materials.

We have compared the different approximations of the BGR for a quantum wire within the RPA and conclude that the plasmon-pole approximation is accurate and that the quasi-static approximation is valid for large densities. Including optical phonons reduces any discrepancies between the different approximations at low densities and increases the BGR slightly for large densities. Including the confinement of the optical phonons

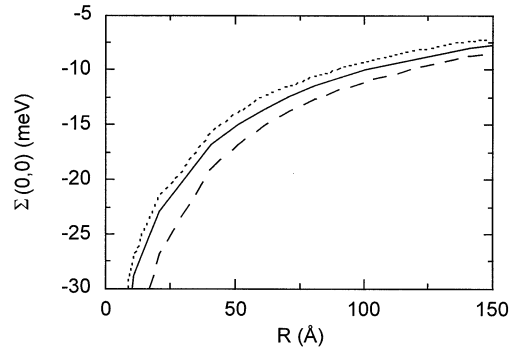


Fig. 2. The bandgap renormalisation against radius R for a GaAs quantum wire embedded in AlAs with a carrier density $n_0 = 10^5 \text{ cm}^{-1}$ using the full result and including bulk GaAs phonons (dashed), bulk AlAs phonons (dotted) and the phonons from the DC model (solid).

produces a result between the BGR using the bulk phonons of each material.

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