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Band-Gap Renormalization in Quantum Wires

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Abstract

Improved techniques in semiconductor fabrication increased the interest in quantum wire structures, because of their opto-electronic device application possibilities. Many-body interactions among the electrons and holes in the wire lead to the band-gap renormalization (BGR), which in turn affect the optical properties of the system. We study the BGR within the random-phase approximation incorporating the dynamical effects, and investigate the density dependence.

Quantum wire structures provide enhanced many-body interactions in a quasi-one-dimensional system to be investigated experimentally. In particular, the band-gap of the wire material, which is an important parameter for the optical and electronic properties of the system, is renormalized by the electrons and holes present and their coupling with the optical phonons in the system. Recent experiments[1] have measured this band-gap renormalization (BGR) for high electron-hole densities produced by photo-excitation[2]. In this work, our aim is to compare various approximations to BGR within the random phase approximation (RPA) and include the effects of bulk phonons.

The self-energy of electrons (holes) at zero temperature is given by

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

BGR is evaluated as the sum of the self-energy of the electrons and holes when $k = 0$ and $\omega = 0$. (We assume equal density for both carrier types.) Eq.(1) may be decomposed into exchange and correlation terms in a standard way[3]. We use the dielectric function in the RPA, together with the Lindhard function $\chi(q, \omega)$,

$$\varepsilon(q, \omega) = \left[1 + \frac{V_{ph}(q, \omega)}{V(q)} \right]^{-1} - V(q) [\chi_e(q, \omega) + \chi_h(q, \omega)], \quad (2)$$

where $V(q)$ is the effective Coulomb potential for cylindrical quantum wire, and $V_{ph}(q) = V(q)(1 - \varepsilon_\infty/\varepsilon_s)\omega_{LO}^2/(\omega^2 - \omega_{LO}^2)$ is the phonon potential, given for the bulk optical phonons. If the phonons are included in the calculation of BGR, the self energy due solely to the phonons should be subtracted, as these are always present. The plasmon pole approximation[4] (PPA) assumes that all of the weight of the dielectric function is at a series of poles. This reduces the dielectric function to,

$$\varepsilon(q, \omega) = \left[1 + \frac{V_{ph}(q, \omega)}{V(q)} \right]^{-1} - \frac{\omega_e^2}{\omega^2 - \omega_{qe}^2} - \frac{\omega_h^2}{\omega^2 - \omega_{qh}^2}. \quad (3)$$

Here $\omega_j^2 = V(q)nq^2/m_j^*$ and $\omega_{qj}^2 = -nq^2/m_j^*\chi_j(q, 0)$. This way, the frequency integral can be evaluated analytically. A further approximation replaces the dielectric function by its static value, and called the quasi-static approximation.

Figure 1 shows the full RPA result, the PPA result, and the result of quasi-static approximation and without bulk GaAs phonons for a GaAs quantum wire. The PPA result moves along the full result, although getting close to the quasi-static result. The quasi-static result over-estimates the BGR for small densities but, as expected, is accurate for large densities. The experiments have been performed, up to now, at these large densities[1]. When the bulk phonons are included, the discrepancy of the quasi-static result at low densities decreases (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.

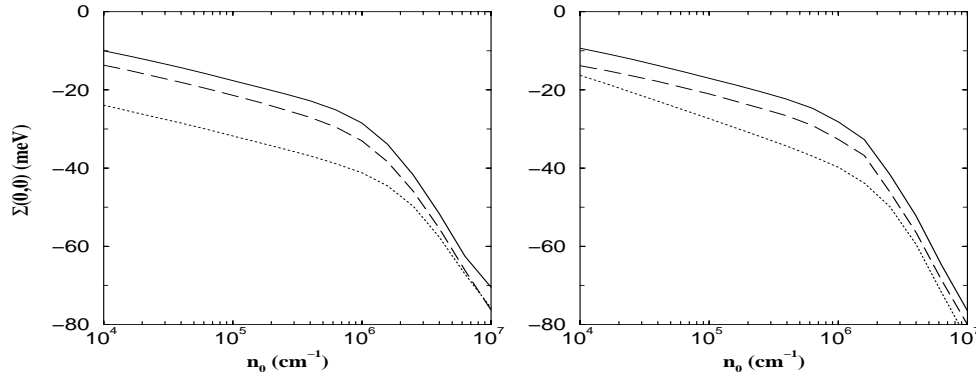


Figure 1. The band gap renormalization as a function of density for GaAs quantum wire of radius $R = 50 \text{ \AA}$ (a) without and (b) with bulk GaAs phonons for the full RPA (solid), the PPA (dashed) and the quasi-static limit (dotted).

Based on these results, we can conclude, within the framework of RPA, that the plasmon-pole approximation is rather accurate, and the quasi-static result is valid for large densities. Including optical phonons reduces the discrepancies among the various approximations considered at low densities, and increases the BGR slightly at large densities.

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