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A numerical study of bandgap narrowing in V-grooved nanowires

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Abstract: We study the effects of higher order excitations on the bandgap renormalization of nano-scale, quasi-one dimensional semiconductor systems within the GW approximation. We incorporate the contribution of the first and the second excited states wave functions in the calculation of the bandgap narrowing which is due to many-body exchange-correlation effects. We show that incorporation of the higher order excitations leads to the result that absolute values of the bandgap narrowing in these cases are larger than the corresponding renormalization calculated just by the ground state wave function.
Keywords : Nanowires, Bandgap Renormalization, GW Approximation.

INTRODUCTION

In recent years, quasi-one dimensional semiconductor quantum wires have been fabricated in a variety of geometric shapes with nano-scale definition, and their optical properties have been studied for potential device applications such as semiconductor lasers [1]. The fundamental gap structure of these quasi-one dimensional systems changes due to the bandgap renormalization (renormalization due to many-body exchange-correlation effects) when many-body effects are taken into account. This effect, as an important nonlinear optical effect in the semiconductor systems, has been studied for different geometries of the confinement potentials (see for instance [2-4] and references therein). Recently, the effect of external electric and magnetic fields on the bandgap renormalization of H-shaped quantum wires has been studied [5]. Here we are going to study the effects of higher order excitations on the bandgap renormalization of the V-shaped quantum wires. By a suitable analytical definition of the quasi-one dimensional V-shaped confinement potential, we use a finite-difference numerical scheme to calculate the eignstates energies and wave functions of charge carriers in the presence of external electric and magnetic fields and for higher order excitations. This analysis will be performed within the Landau gauge for ground state and two first excited states. We obtain the profile of charge carriers distribution (probability amplitudes) in the presence of electric and magnetic fields for these states. Then the many-body exchange-correlation induced bandgap narrowing in this type of quantum wires is studied within the leading order dynamical random phase (GW) approximation. A comparison between the results of different excitations will reveals the role played by higher order excitations in this low-dimensional system.

The confinement potential and Eignstates

The geometry of a typical V-shaped quantum wire is shown in figure 1 where typical values of linear scales are of the order of 50-100 Nm.

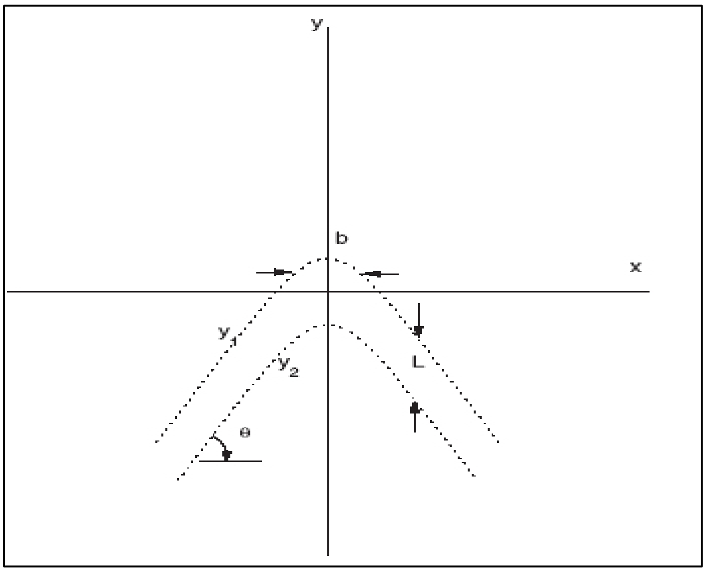

Figure 1. The Geometry of the Confinement Potential

This confinement potential can be described mathematically as follows

$$V(x,y)=\begin{cases} 0 & if \begin{cases} y_2(x)\le x\le y_1(x) \\ y_2(x)\le y\le y_1(x)\end{cases} \\ V_b & elsewhere\end{cases} \quad ....(1)$$

where, from figure 1 we have by definition

$$y_1(x) = -b\tan\theta \ln[\cosh(x/b)] + \frac{L}{2} \quad ......(2)$$

$$y_2(x) = y_1(x) - L \quad ....(3)$$

The effective Schrödinger equation of the system is as follows

$$\left(\frac{d^2}{d\tilde{x}^2}+\frac{d^2}{d\tilde{y}^2}\right)\phi(x,y)-\frac{2mV(x,y)L^2}{\hbar^2}\phi(x,y)=\frac{-2mE(x,y)L^2}{\hbar^2}\phi(x,y) \quad ..(4)$$

where by definition

$$\tilde{x}=\frac{x}{L}\ ,\ \tilde{y}_1(x)=\frac{y_1(x)}{L}\ ,\ \tilde{y}_2(x)=\frac{y_2(x)}{L}$$

We solve this equation numerically to find eignstates of charge carriers in this confinement potential numerically. Figure 2 shows the result of the ground state calculation. These wave functions will be used to calculate the screened Coulomb potential and the bandgap renormalization in next section.

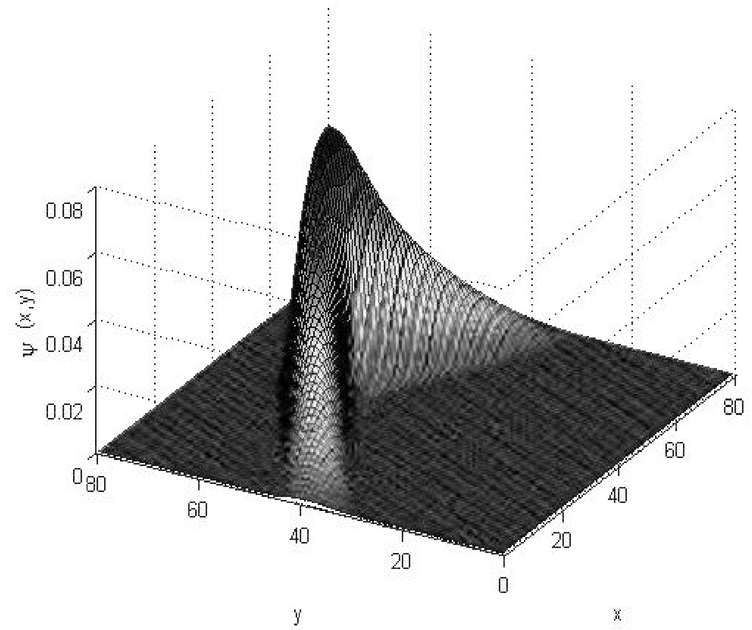

Figure 2. Probability distribution of the ground state

GW Approximation and Bandgap Narrowing

In the GW approximation we have the following Green function

$$G_i(k,z) \cong \frac{1}{z - E_{i,k} - \Delta_i(k) + \mu_i} \quad ....(5)$$

where $\Delta_i(k)$ is the bandgap renormalization due to the many-body exchange-correlation effects. This leads to an effective screening of the Coulomb interaction between electrons and hole which results in a weaker excitonic bound states. By definition, the bandgap narrowing is given by

$$\Delta_i(k) = \Sigma_i\left(k, \varepsilon_{i,k} + \Delta_i(k) - \mu_i\right) \quad .... (6)$$

where up to the first order approximation can be written as

$$\Delta_i(k) = \sum_i (k, E_{i,k} - \mu_i) \quad ....(7)$$

The screened Coulomb interaction is given by

$$V_C(k) = \lambda \frac{2e^2}{\varepsilon_0} L^4 \int d\tilde{x} d\tilde{y} \int d\tilde{x}' d\tilde{y}' K_0 |kR| \; |\phi(\tilde{x},\tilde{y})|^2 |\phi(\tilde{x}',\tilde{y}')|^2 \quad ......(8)$$

Using this screened potential we calculate the bandgap narrowing in this quasi-one dimensional system numerically by using the following relation

$$\Delta_i(k) = \sum_{k'} \left[-V_s(k-k') n_i(\varepsilon_{i,k}) + \frac{1}{2}\left(V_s(k') - V_c(k')\right) \right] \quad ....(9)$$

Where $n_i(E_{i,k}) \equiv (\exp(\beta(E_{i,k} - \mu_i) + 1)^{-1}$ and by definition

$$V_{eff}(k,k',\omega) = \left(\frac{1}{\beta}\right)^2 \sum_{z,z'} \left[\frac{G_e(k,\Omega - z) + G_h(-k,z)}{1 - n_e(\xi_{e,k}) - n_h(\xi_{h,-k})} V_s(k-k', z-z') \times \frac{G_e(k',\Omega - z') + G_h(-k',z')}{1 - n_e(\xi_{e,k'}) - n_h(\xi_{h,-k'})} \right]_{\Omega = \omega - \mu_e - \mu_h + i\delta} \quad ....(10)$$

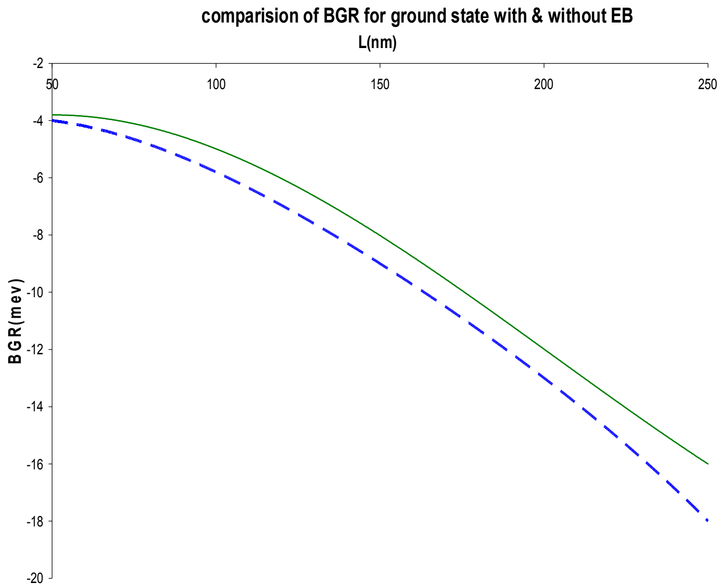

Figure 3. Bandgap narrowing in the presence and absence of Electric and Magnetic fields.

Figure 3 shows the result of our calculations for bandgap narrowing in this quasi-one dimensional system in the presence and absence of Electric and Magnetic fields. In the presence of the EM fields, the bandgap narrowing decreases.

Our treatment shows that bandgap narrowing calculated in GW is larger in magnitude than the value that is calculated through quasi-static approximations. Also the bandgap renormalization calculated from excited states wave functions is larger than those calculated with ground state wave functions.

Conclusion

In this paper, we studied the effect of external electric and magnetic fields and also excited states on the bandgap narrowing in quasi-one dimensional V-shaped nanowires. The presence of the electric and magnetic fields decreases the bandgap narrowing. Also incorporation of the excited states increases the absolute value of bandgap narrowing.

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