

Impurity compensation and band-gap renormalization in double-quantum-wires

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Received 27 April 2004 / Received in final form 23 January 2005

Published online 8 August 2005 – © EDP Sciences, Società Italiana di Fisica, Springer-Verlag 2005

Abstract. We investigate the band-gap renormalization due to electron-electron interaction in the n-type doped GaAs-based double-quantum-wire systems. Electron self-energy is calculated using the leading-order perturbation theory (GW) within the full random-phase-approximation (RPA). We include the impurity effects through Mermin expression and show that decreasing the spacing in double-wire system can compensate partly the undesirable effect of impurities on the band-gap renormalization. Therefore, it is possible to offset the effect of impurity in related devices and to adjust the band-gap. We also, apply a constant electric field to one of the wires. It is shown that the change of the band-gap renormalization in the other wire will be insignificant if the drift velocity does not exceed Fermi velocity.

PACS. 71.10.Ca Electron gas, Fermi gas – 78.67.Lt Quantum wires

1 Introduction

Low-dimensional semiconductors are of great interest in recent years, because of their theoretical values for studying the low-dimensional electron gas systems and also, because of their several important technological applications. The recent progresses in fabrication methods together with the modulation-doping technique, allow tailoring the band structure of the semiconductors and creating the artificial nanostructures such as quasi-one-dimensional electron gas (quantum-wire) in which the motion of electrons is free only in one dimension and quantized in the other dimensions. In quantum-wire systems, the band-gaps can be changed over a wide range, mostly because of the electron-electron interactions. This many-body effect known as the band-gap renormalization can have profound effect on the optical properties of these nanostructures.

It is well known that in extrinsic semiconductors band-gaps are renormalized or narrowed up to tens of meV's due to many-body effects arising from the presence of free carriers in three-dimensional systems [1–15] and two-dimensional systems [16–26]. The band-gap renormalization in single-quantum-wire systems has been studied both experimentally and theoretically by considering electron-electron interaction, electron-phonon coupling, local field correction, wire width, temperature and higher subbands effects [27–36]. Hu and Das Sarma [28] showed the band-gap renormalization in quantum-wires is between 10 to 20 meV. The effects of electron-optical phonon on band-edges of single-quantum-wire based on polar semiconductors have been calculated by Bennett et al. [29]. They

included carrier-carrier and carrier-phonon interactions in self-energy at bandedges of quantum-wire and used three different approaches, RPA approximation, the quasi-static limit and the plasmon-pole approximation, found that confined optical-phonon modes modify the band-gap renormalization. Tanatar [30] has investigated the effect of local-field correction due to the electron correlation on band-gap renormalization in quantum-wires by using Hubbard approximation for the dielectric function. These results compared with the values which were obtained from RPA and it was shown that the local-field correction decreases the band-gap renormalization at low densities and small width (or radius) of the quantum-wires. Tanatar also, calculated the effect of temperature and indicated that the band-gap renormalization in quantum-wire has a weak dependence on temperature. The studies on the effect of finite wire width in quantum-wires systems showed that the band-gap renormalization decreases with increasing the wire width [28, 29]. Higher subbands renormalization in quantum-wires is reported by Wang et al. [31]. They observed a clear dependence of the band-gap renormalization on the subband index through the subband densities.

The band-gap renormalization in double two-dimensional layers has been computed for n-type GaAs-based quantum-wells in reference [26]. The frequency and wave vector dependent RPA dielectric function within leading order GW approximation was applied and it was found that the band-gap renormalization in double layers increases with respect to single layer and more increasing can be obtained by reducing the spacing between two layers. Also, by using Mermin expression, it was shown the undesirable effects of impurity on the band-gap

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renormalization in these systems can be cancelled partly by reducing the spacing between two layers.

The effect of applying an uniform electric field on one of the quantum-wire in double-quantum-wire system has been considered in relation to the drag phenomenon [32].

In this paper, we investigate the band-gap renormalization of the n-type GaAs-based double-quantum-wire, using GW method for self-energy and RPA dielectric function. we have determined the changes of the band-gap renormalization as a function of the electron density, impurity concentration and drift velocity of electrons in one of the wires. In our calculations which are for the lowest subband at zero-temperature, the effects of tunneling between the two wires and electron-phonon coupling are ignored. The effect of impurity scattering is taken into account through Mermin particle-number-conserving expression for susceptibility.

The outline of the paper is as follows. In Section 2.1, we introduce the geometry and the potential formula of our system. Section 2.2 contains the review of the GW formalism, which is used to obtain the changes in self-energies of the conduction and the valence bands. The formalism of the susceptibility and the dynamically screened Coulomb interaction for two parallel electron gas systems (our double-quantum-wire system) are represented in Section 2.3. In Section 2.4 we consider the effects of impurities. In the last part of Section 2, it is shown that the dynamically screened potential in one of the wires will be modified because the electrons in the adjacent wire have non-zero drift velocity. Finally, the results and conclusion are presented in Section 3.

2 Theory

2.1 Model

Our system consists of two parallel equal n-type quantum-wires. We assume each quantum-wire as an one-dimensional electron gas system which is parallel to the x -axis and has an infinite square-well confinement with a finite width a in the y direction and a zero thickness in the z direction. We also, assume one of the wires is placed at $z = 0$ and the other at $z = d$. Along x direction, the electrons move freely without any confinement with parabolic bands so that the unperturbed single-particle energy, $\omega(k)$, is equal to $\hbar^2 k^2 / 2m^*$ where m^* is the band effective mass. The electron wave functions, $\Psi(x, y, z)$, for this infinite square quantum-well, can be obtained from multiplying the envelop function, $f(y, z)$, by the plane wave function, e^{ikx} , where k is a one-dimensional wave vector in x direction. According to the above geometry of the system, the envelop function is obtained by [28,37]:

$$f(y, z) = \phi(y) \sqrt{\delta(z)} \quad (1)$$

where $\phi(y)$ has the following familiar *cosine* or *sine* form [38,39]:

$$\phi(y) = \begin{cases} (2/a)^{1/2} \cos(\pi y/a) & -a/2 < y < a/2 \\ 0 & \text{otherwise.} \end{cases} \quad (2)$$

The electrons in this system interact through Coulomb potential with (i) the other electrons in the same wire which is called intra-wire potential, (ii) the electrons in the adjacent wire that is called inter-wire potential and (iii) the positively charged impurity ions. The electron-impurity interaction can be considered by using Mermin expression for susceptibility of the system (see Sect. 2.4).

The bare Coulomb intra-wire potential, $v(q)$, between the electrons within a single wire is given by [39]

$$v(q) = \frac{2e^2}{\epsilon_0} \int dy \int dy' K_0(|q(y-y')|) |\phi(y)|^2 |\phi(y')|^2. \quad (3)$$

Here ϵ_0 is the background dielectric constant, q is a wave vector along wire axis and $K_0(x)$ is the zeroth-order modified Bessel function of the second kind. For two parallel equal quantum-wires, the bare Coulomb inter-wire potential, $u(q)$, is obtained by [39]:

$$u(q) = \frac{2e^2}{\epsilon_0} \int dy \int dy' K_0 \left(q[(y-y')^2 + d^2]^{1/2} \right) |\phi(y)|^2 |\phi(y')|^2 \quad (4)$$

where d is the separation between two wires. Throughout this paper we ignore the tunneling between two wires by choosing d enough large so that the overlapping between the electron wavefunctions within different wires becomes negligible.

2.2 GW method

In n-type doped semiconductors the extra electrons in conduction band can be delocalized and form an interacting electron gas system. The introduction of the electrons leads to the shifts in the energy of states at the bottom of the conduction band and the top of the valence band so change of the band-gap. By calculating the changes in the self-energy functions of the conduction band, $\Sigma_c(k, \omega)$ and the valence band $\Sigma_v(k, \omega)$, the band-gap renormalization can be obtained. In an interacting system, it is difficult to calculate the self-energy, exactly. However, we use the Hedin's formulation [40] for self-energy which is based on an expansion of the electron self-energy in a perturbative series in powers of the dynamically screened electron-electron interaction, $W(q, \omega)$. The self-energy should in principle be obtained together with dressed Green's function, G , in a self-consistent procedure. In this work, we approximate the self-energy by neglecting vertex correction and taking the leading term in the expansion which is the RPA dynamical screening GW approximation. It has been shown this approach in which non-interacting Green's function, G^0 , is substituted for the interacting one, G , to be used successfully for describing the quasi-particle energies in semiconductors. The self-energy within the GW approximation at $T = 0$ K for a one-dimensional electron gas is given by:

$$\Sigma(k, \omega) = i \int \frac{dq}{2\pi} \int \frac{d\omega'}{2\pi} G^0(k+q, \omega+\omega') W(q, \omega') \quad (5)$$

G_0 , the non-interacting one-electron Green's function, is obtained from [5]

$$G^0(k, \omega) = \frac{1}{\omega - \omega(k) + i\delta \operatorname{sgn}(\omega(k) - \mu)} \quad (6)$$

where $\omega(k)$ is the unperturbed one-particle energy and μ is the chemical potential that is equal to Fermi energy, E_F , at $T = 0$ K. The dynamically Coulomb interaction, $W(q, \omega)$, which introduces the screening effects through the dynamical dielectric function of the electron gas system has been defined by:

$$W(q, \omega) = \frac{V(q)}{\epsilon(q, \omega)} \quad (7)$$

where $V(q)$ is the bare Coulomb potential. In RPA the dielectric function for one-component system is given by

$$\epsilon(q, \omega) = 1 - V(q)\chi^0(q, \omega) \quad (8)$$

where $\chi^0(q, \omega)$ is the non-interacting density-density response function or susceptibility. We calculate the shifts in the self-energy of the conduction and valence bands at each bandedge to get the total change of the band-gap [5]. For n-type GaAs, the change of conduction band is obtained as:

$$\Delta\Sigma_c(k, \omega) = i \int \frac{dq}{2\pi} \int \frac{d\omega'}{2\pi} G_c^0(k+q, \omega+\omega') W(q, \omega'). \quad (9)$$

In definition of G_c^0 , we use $\omega_c(k) = \hbar^2 k^2 / 2m_e^*$ in which m_e^* is the electron effective mass. In confined GaAs, the degeneracy of the heavy hole and the light hole valence bands at $k = 0$ disappears so that the first heavy hole valence subband is the uppermost valence band. The change in the self-energy for valence band can be written as:

$$\Delta\Sigma_v(k, \omega) = i \int \frac{dq}{2\pi} \int \frac{d\omega'}{2\pi} G_v^0(k+q, \omega+\omega') [W(q, \omega') - V(q)]. \quad (10)$$

Here we use $\omega_v(k) = \hbar^2 k^2 / 2m_{\text{hh}}^*$ in calculation of G_v^0 . Using equations (9, 10) we calculate the changes in self-energy of each band at bandedge ($k = 0$) to get the total change of the band-gap.

The shifts in the conduction and the valence bands are due to the changes in both the exchange energy (the new poles of Green's function) and the correlation energy (the poles of the screened Coulomb potential) [41]. In n-type case, there is no contribution from the poles of Green's function in valence band. The total band-gap renormalization is the sum of the changes in the conduction band and the valence heavy hole band, i.e.

$$\Delta E_g = \Delta\Sigma_c(0, 0) + \Delta\Sigma_v(0, 0). \quad (11)$$

This gives a negative value of the total band-gap change when the top of valence band is taken as the origin of the energy [5].

2.3 Two parallel electron gas systems

In this section we present the formalism of two component system to get the band-gap renormalization in a double-quantum-wire system. We consider two adjacent parallel one-dimensional electron gas at zero-temperature. It has been shown that the non-interacting density-density response function for a single-isolated system, $\chi_i^0(q, \omega)$, can be used to construct the generalized susceptibility matrix, χ , for the two-component system [42]. We designate the elements of the generalized susceptibility matrix by $\chi_{ij}(q, \omega)$ where i and j are the component indices. Using RPA, the generalized susceptibility matrix can be written as [42, 43]

$$\chi = [\mathbf{1} - \chi^0 \mathbf{V}]^{-1} \chi^0 \quad (12)$$

where χ^0 is a 2×2 diagonal matrix equals to $\chi_i^0(q, \omega)\delta_{ij}$, and \mathbf{V} is a 2×2 matrix with elements v_{ij} , equal to the bare intra-component potential ($i = j$) and the bare inter-component potential ($i \neq j$). The energy dependent screened potential matrix is given by [42]

$$\mathbf{W} = [\mathbf{1} - \chi^0 \mathbf{V}]^{-1} \mathbf{V}. \quad (13)$$

Therefore the elements of \mathbf{W} are obtained as

$$\begin{aligned} W_{11} &= [\epsilon_{22}(q, \omega) v_{11}(q) + v_{12}(q) \epsilon_{21}(q, \omega)] D(q, \omega) \\ W_{22} &= [\epsilon_{11}(q, \omega) v_{22}(q) + v_{21}(q) \epsilon_{12}(q, \omega)] D(q, \omega) \\ W_{12} &= [\epsilon_{22}(q, \omega) v_{12}(q) + v_{22}(q) \epsilon_{21}(q, \omega)] D(q, \omega) \\ W_{21} &= [\epsilon_{11}(q, \omega) v_{21}(q) + v_{11}(q) \epsilon_{12}(q, \omega)] D(q, \omega) \end{aligned} \quad (14)$$

where $D(q, \omega)$ and $\epsilon_{ij}(q, \omega)$ are defined as

$$D(q, \omega) = \frac{1}{[\epsilon_{11}(q, \omega) \epsilon_{22}(q, \omega)] - [\epsilon_{12}(q, \omega) \epsilon_{21}(q, \omega)]} \quad (15)$$

and

$$\epsilon_{ij}(q, \omega) = \delta_{ij} - v_{ij} \chi_j^0(q, \omega). \quad (16)$$

If we consider two identical electron gas systems, the χ^0 will be a unit matrix times $\chi^0(q, \omega)$ i.e. $\chi_{ij}^0(q, \omega) = \chi^0(q, \omega)\delta_{ij}$. In this case $v_{11}(q) = v_{22}(q) = v(q)$ and $v_{12}(q) = v_{21}(q) = u(q)$ (see Eqs. (3,4)). Using equation (15) for a system with two identical components, the dynamically screened intra-component potential element is given by [42]

$$W_{11}(q, \omega) = \frac{[1 - v(q) \chi^0(q, \omega)] v(q) + [u^2(q) \chi^0(q, \omega)]}{[1 - v(q) \chi^0(q, \omega)]^2 - [u(q) \chi^0(q, \omega)]^2}. \quad (17)$$

We use this effective potential to obtain the band-gap renormalization in each wire.

For a one-dimensional wire the real and the imaginary parts of the non-interacting susceptibility in effective Rydberg unit is given by [44]:

$$\operatorname{Re} \chi^0(q, \omega) = \frac{1}{2\pi q} \ln \left| \frac{\omega^2 - (q^2 - 2qq_F)^2}{\omega^2 - (q^2 + 2qq_F)^2} \right| \quad (18)$$

$$W_{11} = \frac{[1 - v(q)\chi^0(q, \omega - qv_d)]v(q) + u^2(q)\chi^0(q, \omega)}{\{[1 - v(q)\chi^0(q, \omega)][1 - v(q)\chi^0(q, \omega - qv_d)]\} - [u^2(q)\chi^0(q, \omega)\chi^0(q, \omega - qv_d)]}. \quad (22)$$

and

$$\text{Im } \chi^0(q, \omega) = \begin{cases} -1/2q & (q^2 - 2qq_F) < \omega < (q^2 + 2qq_F) \\ 0 & \text{otherwise} \end{cases} \quad (19)$$

where q and q_F are the magnitudes of the wave vector and the Fermi wave vector along the wire axis in effective Bohr radius, respectively.

2.4 Impurity effect

The presence of impurities in semiconductors can have profound effects on the dynamics of the charge carriers. In low dimensional systems the impurity influences the many-body characteristic features of the system. In ideal electron gas, the electrons suffer no collision and have infinite life-time. In n-type doped quantum wire, the free carriers (electrons) are introduced into the system by placing the ionized dopants close to the wire [45]. These dopants can be regarded as weak impurity scattering centers which alter the electron local density and the density response function of the system through the collisional processes and cause the level broadening. In modulation doped quantum wire where there is a spatial separation between the ionized dopants and the electrons, the effects of remote impurities still exist. The bare electron-impurity interaction which has the long-ranged Coulomb interaction nature is screened by the conduction electrons. Therefore, the real electron-impurity interaction should have the short-ranged form and we choose it as $V_{imp}\delta(r - R_i)$ where V_{imp} is the strength of impurity potential and r and R_i are the positions of electron and impurity respectively. For the scattering by the remote impurities, we have assumed that these impurities are located randomly at some distance out of the quantum wire. In this case, the averaged random potential is equal to $N_{imp}V_{imp}^2$ in which N_{imp} is the impurity concentration. There is following relation between this averaged potential and the impurity Born approximation scattering rate or level broadening parameter, γ [28, 46]:

$$\gamma = \frac{1}{2\tau} = \frac{N_{imp}V_{imp}^2}{k_F} \quad (20)$$

where τ is the relaxation time. In one-dimensional electron systems, the existence of impurity scattering centers, changes the non-Fermi liquid behavior of the system to Fermi liquid one [28].

To introduce the effect of the impurities, the standard perturbation theory can be used by including the impurity ladder diagrams into the electron-hole bubble. This leads to a complicated susceptibility, which can be avoided by applying the relaxation-time approximation method. If the effect of finite-relaxation-time is taken into account merely through replacing ω by $\omega + i/\tau$ in susceptibility

function, the local electron density number fails to be conserved [47, 48]. Mermin used a modified relaxation-time approximation in which the collisions between electrons and impurities relax the electronic density matrix to a local equilibrium density matrix. This procedure yields a simple particle-number-conserving expression for susceptibility which contains γ as: [28, 43]

$$\chi^0(q, \omega; \gamma) = \frac{(\omega + i\gamma)\chi^0(q, \omega + i\gamma)}{\omega + i\gamma[\chi^0(q, \omega + i\gamma)/\chi^0(q, 0)]}. \quad (21)$$

We use this expression for our one-dimensional susceptibilities and take γ as an input phenomenological parameter whose value can be obtained from the experimental data for electron mobility, μ_e , through $\gamma = e^2/2m^*\mu_e$. We choose $\gamma \leq E_F$ to ensure the weak impurity scattering process.

2.5 Constant electric field effect

If a constant electric field is applied to one of the wires in double-wire system, the free carriers will move with drift velocity, v_d . This uniform motion of electrons changes their distribution function. The variation of the electron distribution function, in turn, changes the equilibrium susceptibility of the electrons in the wire [49], so the screened intra- and inter-Coulomb interactions will be changed, too. To consider the effect of electron drift in one of the wires on the band-gap of the other wire in a double-quantum-wire system; we introduce the effect of the external constant electric field into the non-interacting susceptibility, $\chi_i^0(q, \omega)$, by shifting the ω to the $\omega - \mathbf{q} \cdot \mathbf{v}_d$ [49]. By using the notation of part 2.2, the screened intra-potential (Eq. (17)), is modified as

See equation (22) above

By inserting this form of screened potential into equations (9,11) we can calculate the band-gap renormalization in a wire when the electrons in its adjacent wire has a finite drift velocity.

3 Results and conclusion

Using equations (9, 11, 18) we have calculated the band-gap renormalization for n-type doped GaAs-based single- and double-quantum-wires systems. In double structures, we have used identical wires. Figure 1 represents the variation of the band-gap renormalization as a function of density parameter, r_s , for one-dimensional single- and double-quantum-wire with damping parameter $\gamma = 10^{-7}E_F$, and spacing $d = 10$ nm. The results indicate that the presence of an adjacent wire increases the band-gap renormalization in each wire. The increase in the band-gap

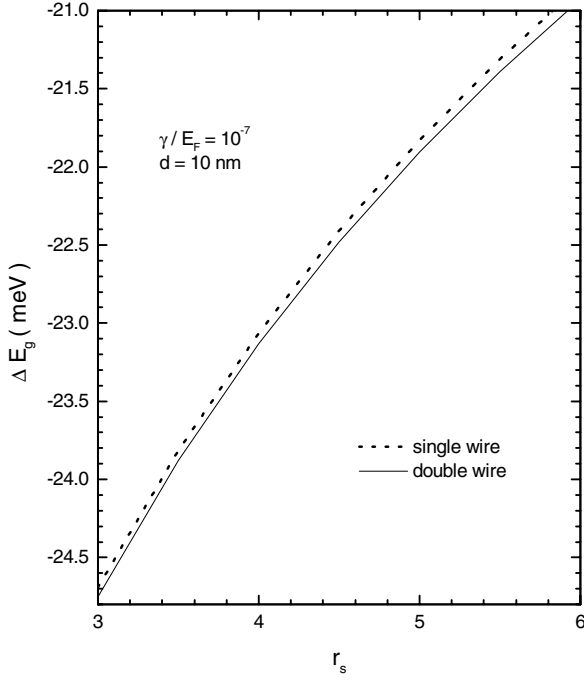


Fig. 1. The band-gap renormalization of one-dimensional single- and double-quantum-wire calculated as a function of the density parameter, r_s , for spacing $d = 10$ nm, and wire width $a = 10$ nm.

narrowing in double-component systems which our numerical results predict, can be explained as follows; the extra carriers in a single-isolated system screen the interaction between the electrons and cause the band-gap reduction. The presence of an adjacent wire introduces further screening causing further reduction in the band-gap. The change in the band-gap renormalization in one wire due to the change in the applied dc electric field (or drift velocity) on the adjacent wire has been verified in double-quantum-wire system. Its results are depicted in Figure 2 as a function of drift velocity for two density parameters, $r_s = 2, 4$. As the Figure 2 shows the band-gap renormalization increases slowly with increasing the drift velocity and this effect is larger for higher densities. We have, also investigated the effects of impurities on double-quantum-wire by changing the corresponding damping parameter, γ , Figure 3. The inclusion of impurity to the system decreases the band-gap renormalization. This is well understood if we notice that the impurity centers which cause the electrons to diffuse instead of moving ballistically, makes the screening strength weaker. In Figure 4, we present the change in band-gap renormalization in double-quantum-wire as a function of damping parameter for spacings equal to 7 nm, 10 nm and 15 nm and for single-isolated quantum-wire. As the results in Figure 4 show increasing the impurity and decreasing the spacing have opposite effects on the band-gap renormalization in double-wire systems. This provides a capability of adjusting the band-gap of quantum-wires, or cancelling the undesirable effects of impurities in the related devices. To

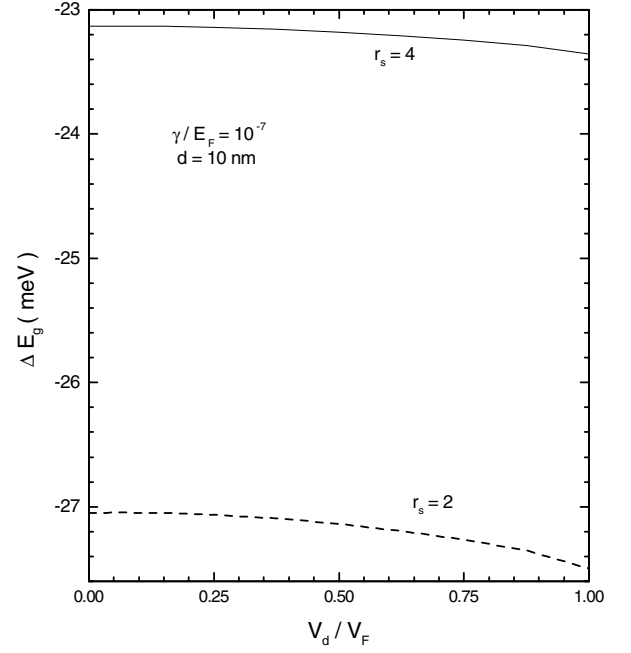


Fig. 2. The band-gap renormalization of double-quantum-wire as a function of the drift velocity for two density parameter, $r_s = 2, 4$, and for wire width 10 nm and spacing $d = 10$ nm.

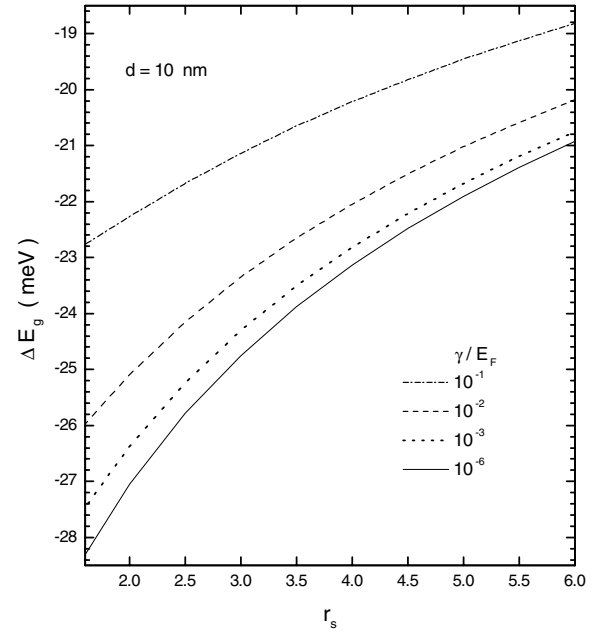


Fig. 3. The band-gap renormalization in one-dimensional double-quantum-wire as a function of density parameter, r_s , with wire width $a = 10$ nm and spacing $d = 10$ nm for different impurity level broadening parameters, γ .

reduce the band-gap about 23 meV in a single-quantum-wire the damping parameter, γ/E_F , must be 10^{-5} , but the same band-gap reduction can be achieved in double-quantum-wire with spacing almost equal to 7 nm having about ten times higher damping parameter, 10^{-4} .

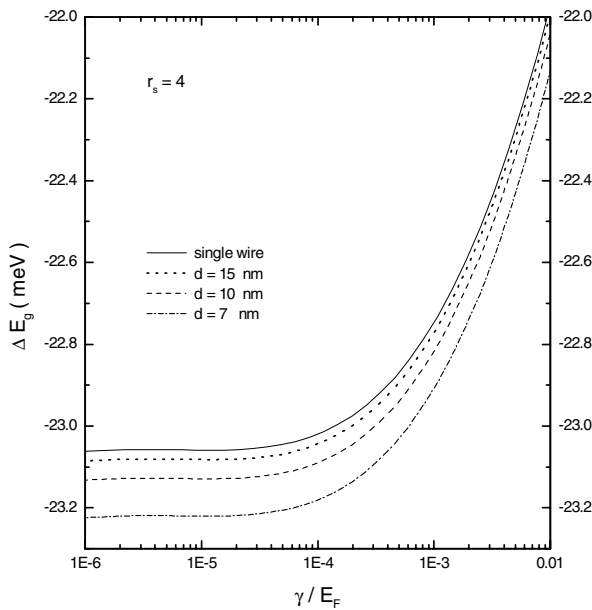


Fig. 4. The band-gap renormalization in one-dimensional double-quantum-wire as a function of impurity parameter, $\gamma/E_F = 10^{-7}$ for different spacings between two wires. The corresponding value for single-isolated quantum-well is also shown. The wire width is 10 nm.

In summary we have calculated the band-gap renormalization for n-type doped GaAs-based double quantum wire system due to the electron-electron interaction at zero temperature using the leading-order perturbation theory (GW) within the full RPA as a function of electron density, spacing between two quantum wires and impurity parameter. We have found the screening effect of the adjacent wire on the band-gap renormalization of the other wire is not very significant; however, it can compensate the undesirable impurity effects by adjusting the spacing between two wires. We have, also, investigated the effect of subjecting one of the wires to a constant and parallel electric field on the band-gap renormalization of the other wire. We have obtained that the band-gap renormalization increases with the increasing of the drift velocity (or electric field strength) and the electron density.

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