

Chemical and magnetic impurity effects on electronic properties of semiconductor quantum wires

Alireza Saffarzadeh*

*Department of Physics, Payame Noor University, Nejatollahi Street, 159995-7613 Tehran, Iran
Computational Physical Sciences Research Laboratory, Department of Nano-Science, Institute for Studies in Theoretical Physics and Mathematics (IPM), P.O. Box 19395-5531, Tehran, Iran*

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We present a theoretical study of electronic states in magnetic and nonmagnetic semiconductor quantum wires. The effects of chemical and magnetic disorder at paramagnetic temperatures are investigated in single-site coherent potential approximation. It is shown that the nonmagnetic impurity shifts the band of carriers and suppresses the van Hove singularities of the local density of states (LDOS) depending on the value of impurity concentration. The magnetic impurity, however, broadens the band which depends on the strength of exchange coupling, and in the high impurity concentration, the van Hove singularities in the LDOS can completely disappear and the curves become smooth.

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I. INTRODUCTION

The nature of the dimensionality and of the confinement associated with a particular nanostructure such as a quantum well, quantum wire, or quantum dot have a pronounced effect on its physical properties. Quantum wires and quantum dots are under active experimental investigation because devices based on them offer important opportunities as the building blocks for the next generation of electronic and optoelectronic devices ranging from ultrafast optical switching to ultradense memories.¹ Quantum wire structures have density of states features which are very useful for laser applications with possibility of smaller current threshold density than in lasers produced from higher dimensional structures. However, it is clear that disorder affects these attractive features of quantum wires.²⁻⁴ Over the past decade, using the coherent potential approximation (CPA), the effects of boundary roughness and the presence of islands on the electronic properties of nonmagnetic semiconductor (NMS) quantum wires have been studied.⁵⁻⁷ Furthermore, it has been demonstrated by Ohno⁸ that it is indeed possible to inject spin from a diluted magnetic semiconductor (DMS) to a NMS, which is necessary in order to carry out qubit (quantum bit) operations required for quantum computing.⁹

DMS's¹⁰ are semiconductors of the general type $A_{1-x}M_xB$, where AB is either a II-VI or a III-V semiconductor and M a magnetic element, most commonly Mn. Substitution of a small fraction x of the element A by Mn impurities (and in the case of II-VI semiconductors an additional charge dopant, such as P on the B site) leads to the appearance of a semiconductor with ferromagnetic properties.^{11,12} The magnetic state in these materials has been attributed to the exchange interaction of the localized Mn moments with the spin of the charge carriers introduced by the Mn dopants, or in the case of II-VI semiconductors, by the additional dopant.

In recent years, considerable works have been devoted to the understanding of physical properties of DMS quantum wires, both theoretically¹³⁻¹⁷ and experimentally.¹⁸⁻²⁰ One of the most important physical quantities in these quantum structures, is the density of states of charge carriers which

depends on the dimensionality of the structure. The behavior of this quantity is very important in determining the electrical, thermal, and other properties of the system. Furthermore, DMS's belong to the class of disordered systems, hence, any first principle consideration should take into account the randomness of impurities. Among different kinds of randomness, two kinds of them can strongly affect the transport properties of charge carriers in DMS quantum wires, i.e., the random substitution of the magnetic atoms and the random direction of the impurity spins.

The aim of this work is to investigate the effects of chemical (spin-independent) potential and magnetic disorder on the electronic properties of semiconductor quantum wires. Based on the single-site CPA for the magnetic and nonmagnetic impurities at paramagnetic temperatures,²¹ we study the local density of states (LDOS) for charge carriers, in terms of the impurity concentrations and spin scattering strengths.

The paper is organized as follows. The model, Hamiltonian and formalism are given in Sec. II. In Sec. III, we present the results of the numerical calculations for the NMS and DMS quantum wires. A brief conclusion is given in Sec. IV.

II. MODEL AND METHOD

We consider a semiconductor quantum wire described by the tight-binding model on a square lattice in which one of the dimensions (the x direction) is much larger than the other (the y direction), i.e., a long-strip lattice in two dimension. The sites of the lattice are denoted by (m, n) where m is an integer number and N_y is number of atoms in the y direction, hence $1 \leq n \leq N_y$. In fact, we have divided the wire into N_y atomic lines along the y axis and each line lies along the x axis. We set the site energies to be infinite along the lines $n=0$ and $n=N_y+1$; thus, the carriers are confined along the y direction. The one-electron Hamiltonian for this system is given by

$$H = \sum_i u_i(M, A) + \sum_{i,j,\sigma} t_{ij} |i, \sigma\rangle \langle j, \sigma|, \quad (1)$$

where u_i depends on whether $i \equiv (m, n)$ is a magnetic (M) or nonmagnetic (A) site. For the A site

$$u_i^A = \varepsilon_A \sum_{\sigma} |i, \sigma\rangle \langle i, \sigma| \quad (2)$$

and for the M site

$$u_i^M = \sum_{\sigma, \sigma'} |i, \sigma\rangle [\varepsilon_M \delta_{\sigma\sigma'} - IS_i \cdot \tau_{\sigma\sigma'}] \langle i, \sigma'|. \quad (3)$$

In the above equations, $|i, \sigma\rangle$ is an atomic orbital with spin σ ($=\uparrow$ or \downarrow) at site (m, n) , ε_A and ε_M are the on-site energies for A and M sites, and the hopping energy $t_{ij}=t$ if i and j are nearest neighbors and zero otherwise. The second term on the right hand side of Eq. (3) is the \mathbf{k} -independent exchange interaction in which \mathbf{S}_i is the local spin operator of the M atom and τ is the usual Pauli matrix for carrier's spin. We regard the spin of magnetic ion as a classical spin, while the value of exchange interaction strength IS ($=I \times S$) is finite.

The single-electron Hamiltonian can be written as

$$H = \mathcal{H}_{\text{eff}} + V, \quad (4)$$

where the effective Hamiltonian \mathcal{H}_{eff} , which describes the effective medium, is expressed as

$$\mathcal{H}_{\text{eff}} = \sum_{i,j,\sigma} [t_{ij} + \delta_{ij} \Sigma_i(\omega)] |i, \sigma\rangle \langle j, \sigma|. \quad (5)$$

Here, $\Sigma_i(\omega)$ is the site-dependent self-energy, and the perturbation term is given as

$$V = H - \mathcal{H}_{\text{eff}} = \sum_i v_i, \quad (6)$$

where $v_i = v_i^A$ for the A site and $v_i = v_i^M$ for the M site are given by

$$v_i^A = \sum_{\sigma} |i, \sigma\rangle [\varepsilon_A - \Sigma_i] \langle i, \sigma|, \quad (7)$$

$$v_i^M = \sum_{\sigma\sigma'} |i, \sigma\rangle [(\varepsilon_M - \Sigma_i) \delta_{\sigma\sigma'} - IS_i \cdot \tau_{\sigma\sigma'}] \langle i, \sigma'|. \quad (8)$$

It should be emphasized that, we have assumed a spin-independent effective medium, since the system is at the paramagnetic temperatures ($T \gg T_c$). Thus, Σ_i does not depend on the spin of carriers and hence, the electronic states will be independent of the temperature within the paramagnetic regime. Here, T_c is defined as the ferromagnetic critical temperature where the spontaneous magnetization of magnetic impurities vanishes, and in $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ quantum wires, for example, T_c as high as 350 K has been reported.²⁰

The matrix elements of effective Green's function \bar{G} can be determined from the Dyson equation

$$\bar{G}_{i,i'}(\omega) = G_{i,i'}^0(\omega) + \sum_j G_{i,j}^0(\omega) \Sigma_j(\omega) \bar{G}_{j,i'}(\omega), \quad (9)$$

where $G_{i,j}^0$ is the clean system Green's function matrix element and is given by

$$G_{i,i'}^0 = \langle m, n | G^0(\omega) | m', n' \rangle = \frac{1}{N_x} \sum_{k_x} \sum_{l=1}^{N_y} \frac{f_{n,n'}(l)}{\omega + i\eta - \epsilon_{l,k_x}} e^{ik_x(m-m')a}, \quad (10)$$

where

$$f_{n,n'}(l) = \frac{2}{N_y + 1} \sin\left(\frac{l\pi}{N_y + 1}n\right) \sin\left(\frac{l\pi}{N_y + 1}n'\right) \quad (11)$$

and

$$\epsilon_{l,k_x} = 2t \cos\left(\frac{l\pi}{N_y + 1}\right) + 2t \cos(k_x a) \quad (12)$$

is the clean system band structure.

Here, N_x and k_x are the number of lattice sites and the wave vector in the x direction, a is the lattice constant, l is the mode of the subband, and η is a positive infinitesimal. Since the translational symmetry is absent in the y direction, the self-energy depends on the atomic line number (n), however, it is independent of the number (m) of the atomic site on each line, i.e., $\Sigma_i(\omega) \equiv \Sigma_n(\omega)$. In this case, the Dyson equation (9) can be rewritten as

$$\begin{aligned} \bar{G}_{n_1, n_2}(m_1, m_2; \omega) &= G_{n_1, n_2}^0(m_1, m_2; \omega) + \sum_{n=1}^{N_y} \sum_m G_{n_1, n}^0(m_1, m; \omega) \\ &\times \Sigma_n(\omega) \bar{G}_{n, n_2}(m, m_2; \omega). \end{aligned} \quad (13)$$

The CPA replaces the real system with an effective periodic medium.^{22,23} For this purpose, the potential of all sites is replaced by an energy-dependent coherent potential, except one site which is denoted by impurity. The effective medium is determined self-consistently in such a way that the Green's function of the effective medium is equal to the configurationally averaged Green's function of the real medium. Therefore, the effective scattering of a carrier at the impurity site is zero, on average.

In order to derive the CPA equation for the coherent potential, we write the Green's function of the real system $G \equiv (\omega - H)^{-1}$ in terms of the effective Green's function \bar{G} and the total scattering matrix T as

$$G = \bar{G} + \bar{G} T \bar{G}, \quad (14)$$

where $T = V(1 - \bar{G}V)^{-1}$. Using the multiple scattering theory,²³ one can express T as the multiple scattering series

$$T = \sum_i t_i + \sum_i \sum_{j \neq i} t_i \bar{G} t_j + \sum_i \sum_{j \neq i} \sum_{k \neq j} t_i \bar{G} t_j \bar{G} t_k + \dots \quad (15)$$

Here, $t_i (\equiv t_{m,n})$ is the single-site t matrix which represents the multiple scattering of carriers due to the isolated potential $v_i (\equiv v_{m,n})$ in the effective medium, and is expressed as

$$t_i = v_i (1 - \bar{G}v_i)^{-1}. \quad (16)$$

The averaging of Eq. (14) and the use of single-site CPA condition $\langle t_i \rangle_{\text{av}} = 0$ for any site i in the wire, leads to $\langle T \rangle_{\text{av}} = 0$ and thus, we obtain $\langle G \rangle_{\text{av}} = \bar{G}$, as mentioned above.

The present system includes both substitutional disorder and spin scattering. Therefore, the CPA equation for the coherent potential is given by

$$\langle t_{m,n} \rangle_{\text{av}} = (1-x)t_{m,n}^A + x\langle t_{m,n}^M \rangle_{\text{spin}} = 0, \quad (17)$$

where $t_{m,n}^A(t_{m,n}^M)$ represents the complete scattering associated with the isolated potential $v_{m,n}^A(v_{m,n}^M)$ in the effective medium and $\langle \cdots \rangle_{\text{spin}}$ denotes average over the spin scattering at the M site. In the classical spin treatment, the potential for which a carrier is subjected at the M site is regarded as $\varepsilon_M - IS$ or $\varepsilon_M + IS$, depending on whether the localized spin on the M site and the carrier spin are parallel or antiparallel with each other. At the paramagnetic temperature at which the orientation of localized spin is completely random, the probability of each state is $1/2$. Therefore, the associated t matrices for an arbitrary site of each atomic line, such as $(0, n)$, are given by

$$t_{0,n}^A = \frac{\varepsilon_A - \Sigma_n}{1 - (\varepsilon_A - \Sigma_n)F_n} \quad (18)$$

and

$$\begin{aligned} \langle t_{0,n}^M \rangle_{\text{spin}} = & \frac{1}{2} \left[\frac{\varepsilon_M - IS - \Sigma_n}{1 - (\varepsilon_M - IS - \Sigma_n)F_n} \right] \\ & + \frac{1}{2} \left[\frac{\varepsilon_M + IS - \Sigma_n}{1 - (\varepsilon_M + IS - \Sigma_n)F_n} \right], \end{aligned} \quad (19)$$

where

$$\begin{aligned} F_n(\omega) &= \bar{G}_{n,n}(m, m; \omega) \\ &= \bar{G}_{n,n}(0, 0; \omega) = \frac{a}{2\pi} \int_{-\pi/a}^{\pi/a} \bar{G}_{n,n}(k_x; \omega) dk_x \\ &\text{for } n = 1, \dots, N_y. \end{aligned} \quad (20)$$

In Eq. (20), we should emphasize that the effective Green's function, \bar{G} , depends on the one-dimensional wave vector k_x via G^0 [see Eq. (10)]. Hence, to obtain any specific matrix element \bar{G}_{n_1, n_2} , we must integrate over the first Brillouin zone of the one-dimensional lattice.²³

Equation (17) leads to a cubic equation for the self-energy of n th atomic line $\Sigma_n(\omega)$ as

$$A\Sigma_n^3 + B\Sigma_n^2 + C\Sigma_n + D = 0 \quad \text{for } n = 1, \dots, N_y, \quad (21)$$

with

$$A = -F_n^2, \quad (22)$$

$$B = (\varepsilon_A + 2\varepsilon_M)F_n^2 - 2F_n, \quad (23)$$

$$\begin{aligned} C = & [(IS)^2 - 2\varepsilon_A\varepsilon_M - \varepsilon_M^2]F_n^2 + [x(\varepsilon_M - \varepsilon_A) \\ & + 2(\varepsilon_M + \varepsilon_A)]F_n - 1, \end{aligned} \quad (24)$$

$$\begin{aligned} D = & [\varepsilon_M^2\varepsilon_A - (IS)^2\varepsilon_A]F_n^2 + [x(IS)^2 + (x-2)\varepsilon_M\varepsilon_A - x\varepsilon_M^2]F_n \\ & + x(\varepsilon_M - \varepsilon_A) + \varepsilon_A. \end{aligned} \quad (25)$$

It should be noted that, Eq. (13) is a system of linear equations which should be solved self-consistently, using Eqs. (20) and (21), to obtain the coherent potentials $\Sigma_n(\omega)$. Then, the LDOS per site in the n th atomic line of the quantum wire, $g_n(\omega)$, is calculated by

$$g_n(\omega) = -\frac{1}{\pi} \text{Im } F_n(\omega). \quad (26)$$

We should remind the reader that the LDOS is a function of the energy and the space coordinate, which illustrates the spatial distribution of the states at the particular location (here, n), and it is well known that many important physical properties and characteristics of a mesoscopic system are determined by the LDOS, which is experimentally measurable.

When Eq. (21) is solved for a real energy ω , we obtain three roots. We only choose the correct root corresponding to $\omega + i\eta$, i.e., the imaginary part of F_n must be negative in order to give a positive LDOS. The existence and uniqueness of such a solution depend on the initial guess for the self-energies Σ_n . We believe that the best guess for Σ_n is zero. One should note, however, that the real and imaginary parts of the roots and the speed of convergence depend on the parameters of the system. Except for a few values of the energy, we have rapid convergence when the final value of Σ_n for a given energy is taken as the initial Σ_n for the next energy. Furthermore, in the case of weak exchange interaction, the convergence is faster than in the strong one.

It is important to note that, if we set $IS=0$, the present formalism will be applicable for a NMS quantum wire of general type $A_{1-x}D_xB$ which has been doped with donor or acceptor nonmagnetic impurities. Here, D indicates the nonmagnetic impurity atom, and in the above equations, we should set $\varepsilon_M = \varepsilon_D$. In next section we present the numerical results of LDOS for both the NMS and DMS quantum wires.

III. RESULTS AND DISCUSSION

In our numerical calculations, we measure the energies in units of t and we set $\varepsilon_A=0$, since we can shift the chemical potential without loss of physics. We present the numerical results for both the NMS and DMS quantum wires with $N_y=5$. In both cases, we have assumed the carrier density is very low; hence, we have ignored the interaction between carriers. In practice, we have done the numerical calculations for a case in which only single carrier moves in the conduction (or valance) band of the quantum wire.

In quantum wires, quantum effects influence the electronic properties of the system. Due to the confinement of free carriers in the transverse direction of the wire, their transverse energy is quantized into a series of discrete values. In practice, when the size or dimension of a material diminishes to the nanoregion, the charge carriers begin to experience the effects of confinement, meaning that their motion becomes limited by the physical size of the region or domain in which they move.

In Fig. 1, the energy dispersion and the LDOS curves of a clean quantum wire are shown for comparison. In such system, there are states with zero group velocity which are re-

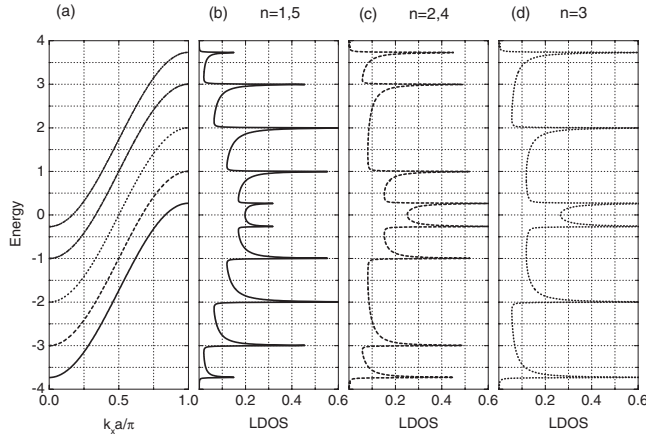


FIG. 1. The energy dispersion and the LDOS curves of a clean semiconductor quantum wire. (a) The dispersion curve as a function of normalized wave vector and (b)–(d) the LDOS as a function of energy, for the atomic lines $n=1,5$, $n=2,4$ and $n=3$, respectively. Energy is measured in units of t .

sponsible for the singularities of spectral density. Therefore, the van Hove singularities appear as sharp features in the LDOS and due to the presence of five atomic lines, five subbands are observed.²⁴ Due to the symmetry of the system, the LDOS for $n=1$ is the same as for $n=5$ (which are at the edges of wire), and $n=2$ with $n=4$. Also, the number of sharp peaks depends on the atomic line number.

To illustrate the impurity effects in NMS quantum wires, the LDOS as a function of energy is plotted in Fig. 2 for $\varepsilon_D = -0.75$ and in Fig. 3 for $\varepsilon_D = +0.75$. An impurity with negative (positive) site energy is analogous to an acceptor (a donor) center at the host crystal. At zero concentration of impurity ($x=0$), the band for all atomic lines, is equivalent to the one in the clean system [see Figs. 1(b)–1(d)]. For the case of $\varepsilon_D < 0$ ($\varepsilon_D > 0$), with increasing x the band shifts towards lower (higher) energies. Also, with increasing x , the relative sharpness of peaks reduces and at $x=0.5$ which represents the state of maximum substitutional disorder, the LDOS is completely symmetric with respect to the center of band and the sharpness disappears. With further increasing x , the peaks again become sharp, and for $x=1$, the LDOS with a shift equal to ε_D , is completely equivalent to the band of clean system. The reason of such behavior is that, for $x > 0.5$ the majority of atoms have $\varepsilon_D \neq 0$ ($\varepsilon_D = -0.75$ or $\varepsilon_D = +0.75$ depending on the type of impurity). Thus, one can imagine the situation in which the atoms with $\varepsilon_D = 0$ act as impurity atoms in a host crystal with $\varepsilon_D \neq 0$. These features can be seen in all atomic lines. Therefore, the nonmagnetic impurity can change the behavior of LDOS and there is not band broadening in the NMS quantum wires.

We now investigate the influence of magnetic impurities on the electronic properties of semiconductor quantum wires. Doping of magnetic atoms such as Mn into GaAs or InAs quantum wires, introduces not only magnetic moments but also free carriers. Therefore, in such quantum wires, we should consider both the effects of chemical potential and magnetic disorder on the LDOS at the paramagnetic temperatures. Figures 4 and 5 show how the carrier band

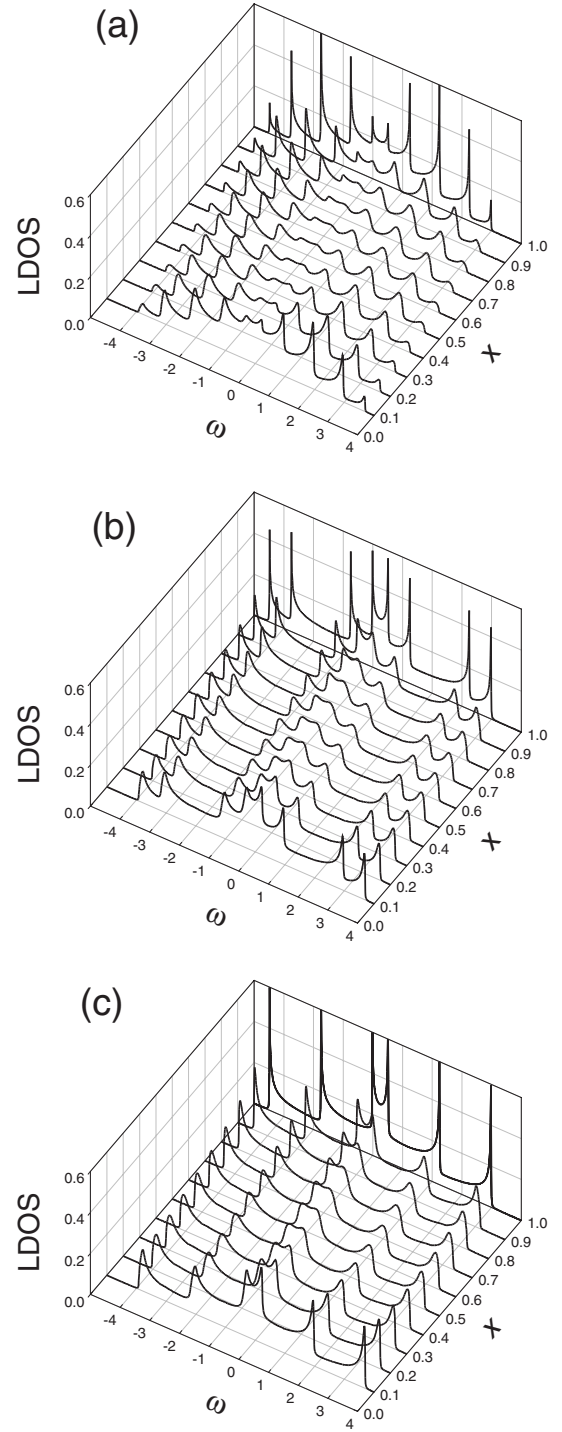


FIG. 2. The LDOS of a NMS quantum wire with $\varepsilon_D = -0.75$ as functions of energy and impurity concentration, for the atomic lines (a) $n=1,5$, (b) $n=2,4$, and (c) $n=3$, respectively. Energy is measured in units of t .

changes with x in the case of weak and strong exchange interaction, respectively. We have shown the results for $\varepsilon_M = -0.75$, $IS = -0.4$ (weak exchange interaction), and $IS = -1.2$ (strong exchange interaction) as sampling cases of III-V-based DMS's. For this kind of impurity, with increasing x the sharpness of peaks decreases continuously and at the concentration $x=1.0$ at which the LDOS is completely sym-

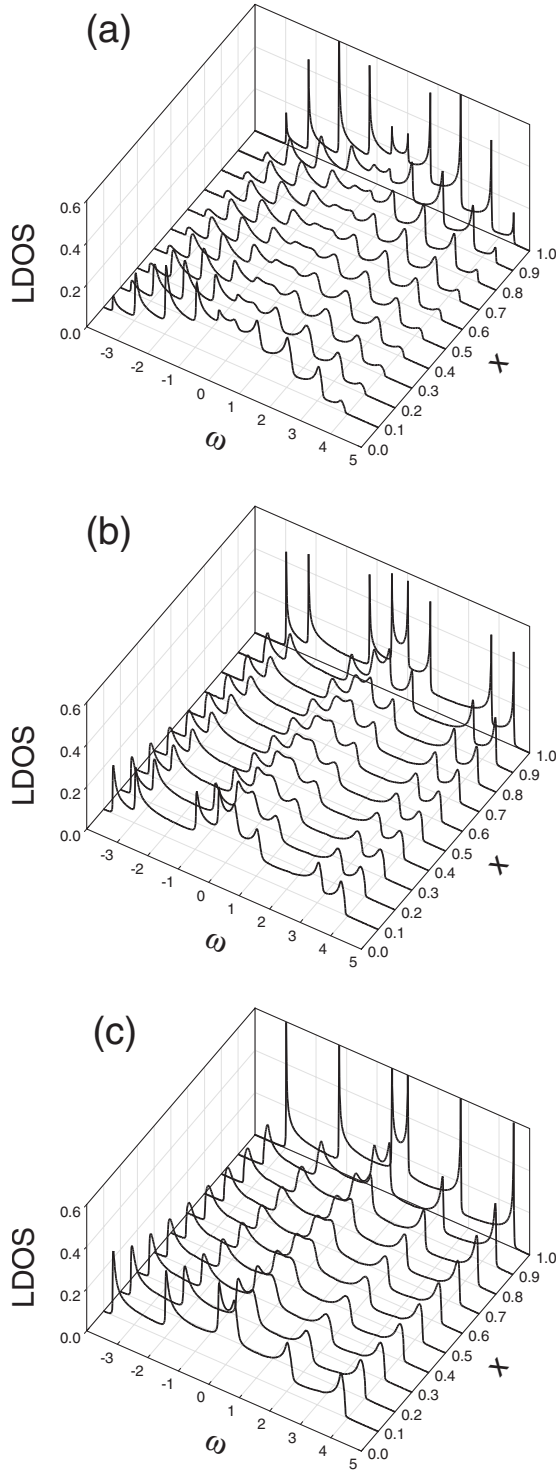


FIG. 3. The same as Fig. 2 but for $\varepsilon_D = +0.75$.

metric with respect to the center of band, the van Hove singularities completely disappear (particularly for $IS = -1.2$), and the curves of all atomic lines become smooth. Such features have not been observed in the bulk case.²¹ It should be noted that the results are same for different signs of IS , because the system is in paramagnetic phase and the spin of magnetic atoms is treated classically.

On the other hand, the results show that, the LDOS of atomic lines is different with each other. This feature indi-

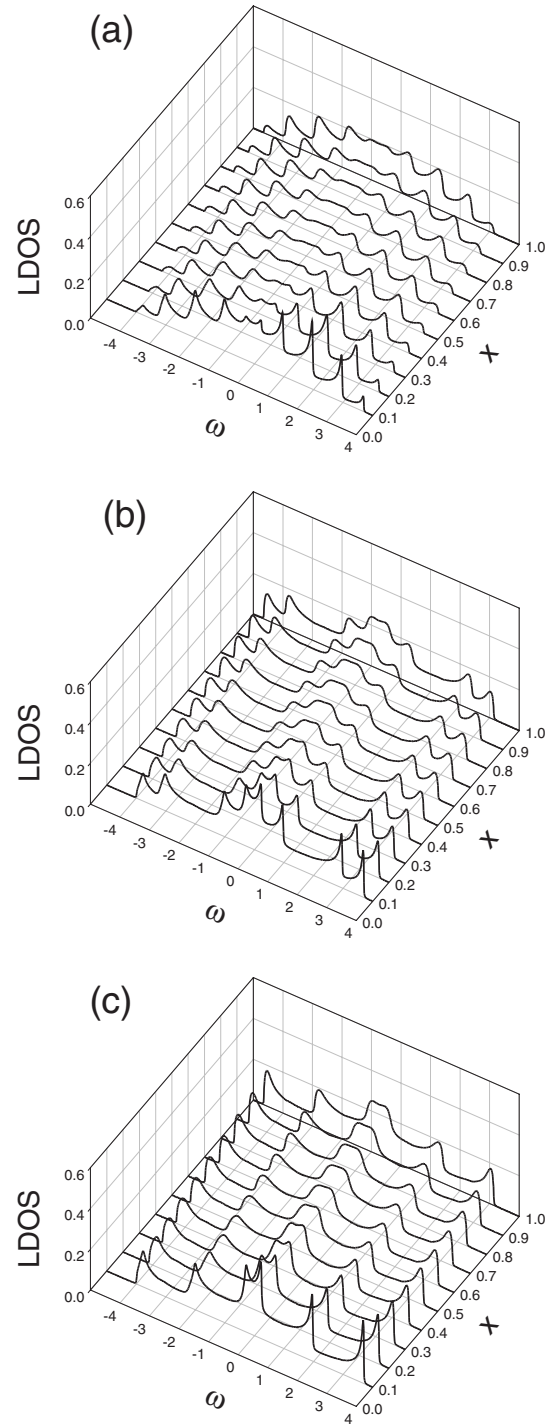
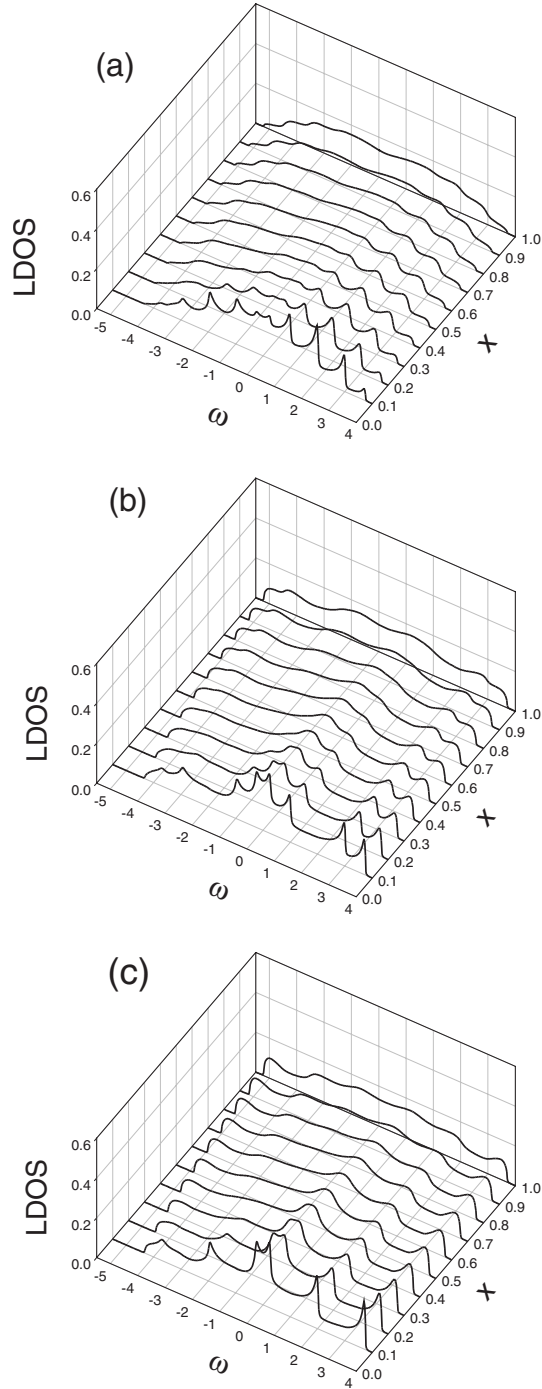


FIG. 4. The LDOS of a DMS quantum wire with $\varepsilon_M = -0.75$ and $IS = -0.4$ as functions of energy and impurity concentration, for the atomic lines (a) $n=1, 5$, (b) $n=2, 4$, and (c) $n=3$, respectively. Energy is measured in units of t .

cates that the electronic transport depends on the atomic line number. The difference in the density of states of the atomic lines predicts a nonuniform charge distribution in such quantum wires. Therefore the atomic lines will have different contributions in carrier transport and cause the quantum interferences, which can be important in the process of charge transport through nano-scale devices. Similar feature in the

FIG. 5. The same as Fig. 4 but for $IS = -1.2$.

coherent electron conductance of a quantum point contact in the presence of a scanning probe microscope tip, has been reported both experimentally²⁷ and theoretically.²⁸

Now, we discuss the band-edge energy shift and the band broadening due to the random distribution of M ions and the fluctuation of localized spins. The energy shift and the broadening of the band can be calculated using the band-edge energies ω_b at which the density of states goes to zero and the imaginary part of the self-energy vanishes. The approximate solution for the lower (upper) band edge is given by²¹

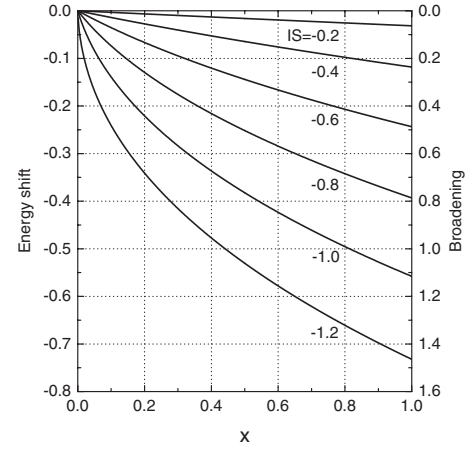


FIG. 6. The energy shift of the lowest band edge and the band broadening for various values of IS , with $\varepsilon_M = 0$ as a function of impurity concentration. Energy is measured in units of t .

$$\omega_b = \Sigma_n^{l(u)}(\omega_b) \mp W_0, \quad (27)$$

where $\Sigma_n^{l(u)}(\omega_b) \equiv \Sigma_b^{l(u)}$ is the energy shift of the lower (upper) band edge, and $W_0 \approx 3.74t$ is the half-bandwidth of the clean system. Using Eqs. (20) and (27), we numerically obtain $F_n(\omega_b)t \approx \mp 0.81$. Substituting these values into Eq. (21), we obtain real $\Sigma_b^{l(u)}$ or the energy shifts of the band edges for the system. In Fig. 6, the band-edge energy shift and the band broadening are depicted as a function of the impurity concentration for various values of IS , with $\varepsilon_M = 0$ for simplicity. In such a case, the LDOS is symmetric around $\omega = 0$, hence the magnitudes of the band-edge energy shifts are equal and the band broadening is given by $2|\Sigma_b^l|$ or $2|\Sigma_b^u|$. The results clearly show that, in the presence of magnetic impurities, the bands are broadened with the increase of x due to the impurity spin fluctuation. This band broadening depends on the strength of magnetic disorder and is much larger when the interaction is stronger (compare Figs. 4 and 5).

We applied our theory for both the NMS and DMS quantum wires, by employing parameters for simulating the semiconducting alloys. The parameters of the tight-binding model used in this work can be chosen from realistic orbitals of atomic species which are suitable for an experimental realization of the modeled quantum wires. Such parameters have been used to study bulk DMS's.^{21,25} However, we should note here that, our investigation is based on a single-band model and a single-site approximation, neglecting many features such as multiband effects, off-diagonal disorder, Coulomb interactions between free carriers, and correlated defects. If such features affect the physical properties of a real system, the above mentioned model should be improved. Otherwise, one cannot expect to obtain accurate results for that system, using the experimental parameters.

One could consider the present system as an infinite stack of atomic slices along the x direction. This means that we consider the disorder in the y direction. Thus, in such a case, we should define a position-dependent self-energy for each slice. In other words, the self-energy, in the cross section of

the wire, is different from one site to the other; however, the slices have equal self-energy values. The single-site CPA condition should be used for each slice to obtain the self-energies, and, in order to derive the Green's function of such a system, one can use a method similar to that for semi-infinite leads.^{5,6,26}

The calculations presented here can be extended for more than one atomic strip and study the transport of free carriers parallel to the strips (layers). In such a case, the transport properties of the system depend on the strip number, which can be attractive for planar devices with submicron dimensions.

IV. CONCLUSIONS

We have studied the effects of magnetic and nonmagnetic impurities on the electronic states of semiconductor quantum

wires. Using the CPA for random distribution of impurity atoms, we investigated the influence of impurity concentration and the strength of exchange interaction on the LDOS. In NMS quantum wires, the acceptor (donor) impurities only shift the bands towards lower (higher) energies, and the van Hove singularities in the LDOS depend on the value of impurity concentration. For DMS quantum wires, the magnetic impurities broaden the bands and reduce continuously the peaks sharpness, even in the case of weak exchange coupling. The results presented here predict that the DMS quantum wires can be used in laser operation and the physics of spintronic nanodevices.

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*a-saffar@tehran.pnu.ac.ir

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