Theoretical investigation of excitons in type-I and type-II Si/Si$_{1-x}$Ge$_x$ quantum wires

J. Costa e Silva,* Andrey Chaves,† J. A. K. Freire,‡ V. N. Freire, and G. A. Farias§
Departamento de Física, Universidade Federal do Ceará, Caixa Postal 6030, Campus do Pici, 60455-900 Fortaleza, Ceará, Brazil
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This work presents a theoretical study of the excitonic properties of Si$_{1-x}$Ge$_x$ cylindrical quantum wires surrounded by a Si matrix, considering two possibilities for the conduction band alignment, type I and type II. The effect of nonabrupt interfaces between these materials on the exciton energies is investigated: an interfacial region of 15 Å in a 50 Å wide Si$_{0.85}$Ge$_{0.15}$(Si$_{0.7}$Ge$_{0.3}$) type-I (type-II) quantum wire leads to an exciton energy blueshift of the order of 10 meV. The excitonic behavior under an applied magnetic field parallel to the wire axis is also studied: exciton energies in type-I wires are weakly affected, while for type-II wires, increasing the field causes the electron angular momentum to change almost periodically, giving rise to Aharonov-Bohm oscillations of the exciton ground state energy.

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I. INTRODUCTION

Over the past few years, many researchers have studied one-dimensional nanoscale structures such as quantum wires (QWR), due to their potential applications in electronic devices, e.g, transistors, diodes, lasers, and biological sensors, and also because their chemistry is quite easily manipulated.[1–3] Many groups have used several growth techniques to synthesize QWR composed of two single-crystalline semiconductor materials, forming core-sheath, core-multishell, and block-by-block heterostructures.[4–6] In particular, recent papers have reported the growth of Si/SiGe QWR by using *chemical vapor deposition* and *vapor liquid solid deposition* methods, which exhibit enhanced electrical transport properties making possible high-mobility devices.[4,7]

Experimental studies on Si$_{1-x}$Ge$_x$ quantum wells, wires, and dots surrounded by a Si matrix have indicated that such heterostructures exhibit a peculiar characteristic of their band structure: the valence band always forms a well for holes, whereas there are two possible kinds of band alignment for electrons, depending on the Ge concentration x. It has been shown that for low Ge concentrations, the conduction band forms a well (type I) for electrons, while at higher concentrations it may form a barrier (type II).[8–12]

There are many papers in the literature related to excitons in type-II quantum dots and wells. Although the exciton confinement in type-II wires is also an interesting problem, there have been few theoretical works on this subject. Rorison[13] was one of the first ones to present theoretical studies of excitonic properties of type-II QWR systems, in which exciton binding energies and oscillator strengths were calculated for GaAs/AlAs QWR, for both finite and infinite confining barrier cases, using a variational approach and a self-consistent method. However, his work did not study how the excitonic properties of these systems may be affected by the presence of external magnetic fields. Recently, the problem of exciton confinement was addressed for type-II planar quantum dots under an applied magnetic field, perpendicular to the dot plane, by Janssens *et al.*,[14] where interesting results were found about the angular momenta of carriers in the ground state for high fields. The influence of magnetic fields on the exciton states in QWR has also been widely studied,[15–19] but mainly in type-I systems.

Another important topic is the influence of an interfacial layer between Si and SiGe on the calculation of exciton energies, since in almost all recent experimental publications, the composition analysis of the wires indicates the presence of nonabrupt interfaces between materials. The problem of graded interfaces in low dimensional systems, such as quantum dots and quantum wells, has been widely studied, and significant alterations of the exciton energy spectrum have been demonstrated.[20–22]

The aim of the present work is to study the excitonic properties of Si$_{1-x}$Ge$_x$ cylindrical quantum wires embedded in a silicon matrix. We consider the two known possibilities for band alignment in these systems, type I and type II, for appropriate Ge compositions. Taking into account the existence of graded interfaces, the effective mass approximation is used to calculate the exciton energies. The electron and hole behaviors under an applied magnetic field parallel to the wire axis are also investigated, showing Aharonov-Bohm (AB) oscillations of the electron ground state energies of type-II Si/Si$_{1-x}$Ge$_x$ QWR.

II. THEORETICAL MODEL

Considering the symmetry of the problem, circular cylindrical coordinates are used, taking ρ as the confinement direction and z as the free direction. Using the symmetric gauge for the vector potential, $\mathbf{A}=\frac{1}{2}B\rho\hat{e}_\theta$, the Hamiltonian that describes the system is given by[25]

$$H_{exc}=-\frac{\hbar^2}{2}\left[\frac{1}{\rho_i}\frac{\partial}{\partial\rho_i}\left(\frac{\rho_i}{m_i^{\parallel}(\rho_i)}\frac{\partial}{\partial\rho_i}\right)+\frac{1}{m_i^{\parallel}(\rho_i)\rho_i^2}\frac{\partial^2}{\partial\theta^2}+\frac{1}{\mu_\perp}\frac{\partial^2}{\partial z^2}\right]-\frac{i}{2}\hbar\omega_c\frac{\partial}{\partial\theta}+\frac{1}{8}m_i^{\parallel}\rho_i^2\omega_c^2+V_i(\rho_i), \quad (1)$$

where $i=e$, h, $m_i^{\parallel}$ is the in plane ρ-dependent effective mass of each charge carrier, $\mu_\perp$ is the electron-hole reduced mass in the z direction, and $\omega_c=eB/m_i^{\parallel}$ is the cyclotron angular frequency. We use the relative coordinates $z=|z_e-z_h|$ and $\theta=\theta_e-\theta_h$. The potential $V_i(\rho_i)$ includes the heterostructure potential $V_i^{het}(\rho_i)$ and the Coulomb interaction between electrons and holes.

To take into account the existence of a graded interface between materials, the Ge concentration χ of the alloy is assumed to be ρ-dependent, similar to the model of Freire *et al.*[23] For a $\chi(\rho_i)$ increasing linearly in the interfacial region, one has

$$\chi(\rho_i)=\begin{cases} x, & 0\leqslant\rho_i<\rho_1; \\ x-(\rho_i-\rho_1)x/w, & \rho_1\leqslant\rho_i<\rho_2; \\ 0, & \rho_i\geqslant\rho_2, \end{cases}$$

where ρ_1 and ρ_2 are the limits of the interfacial region and $w=\rho_2-\rho_1$ is the interface thickness. $V_i^{het}(\rho_i)$ and $m_i^{\parallel}(\rho_i)$ are then expressed as functions of $\chi(\rho_i)$: $V_i^{het}(\rho_i)=Q_i[\epsilon_1\chi(\rho_i)+\epsilon_2\chi^2(\rho_i)]$ and $m_i^{\parallel}(\rho_i)=\{m_{i,\mathrm{Ge}}\chi(\rho_i)+m_{i,\mathrm{Si}}[1-\chi(\rho_i)]\}$, where ϵ_1 and ϵ_2 are interpolation parameters and Q_i is the band offset.[8]

The eigenfunction which is the solution in the θ coordinate is chosen as $(1/\sqrt{2\pi})e^{il\theta}$, where $l=0,\pm1,\pm2,\ldots$, is the angular momentum. Using a variational approach, we take a Gaussian-type "orbital" wave function[24] as the solution in z

$$\phi(z)=\frac{1}{\sqrt{\eta}}\left(\frac{2}{\pi}\right)^{1/4}\exp\left(-\frac{z^2}{\eta^2}\right), \tag{2}$$

with η as the variational parameter that minimizes the exciton binding energy.

For type-I systems, it is used for the exciton wave function $\Psi(\rho_e,\rho_h,\theta,z)=(1/\sqrt{2\pi})e^{il\theta}\psi_e(\rho_e)\psi_h(\rho_h)\phi(z)$, where ψ_e and ψ_h are normalized one particle wave functions, in the Schrödinger equation with the Hamiltonian of Eq. (1), namely $\langle\Psi|H_{exc}|\Psi\rangle=E_x\langle\Psi|\Psi\rangle$. Thus,

$$E_x=\langle\psi_e|H_e|\psi_e\rangle+\langle\psi_h|H_h|\psi_h\rangle+\langle\Psi|H_{e\text{-}h}|\Psi\rangle, \tag{3}$$

where the one particle Hamiltonian H_i is given by

$$H_i=-\frac{\hbar^2}{2\rho_i}\frac{\partial}{\partial\rho_i}\left(\frac{\rho_i}{m_i^{\parallel}(\rho_i)}\frac{\partial}{\partial\rho_i}\right)+\frac{\hbar^2l^2}{2m_i^{\parallel}(\rho_i)\rho_i^2}+\frac{l}{2}\hbar\omega_c + \frac{1}{8}m_i^{\parallel}(\rho_i)\omega_c^2\rho_i^2+V_i^{het}(\rho_i) \tag{4}$$

with i=, e, h, and H_{e-h} is the electron-hole interaction Hamiltonian

$$H_{e\text{-}h}=-\frac{\hbar^2}{2\mu_\perp}\frac{\partial^2}{\partial z^2}-\frac{e^2}{4\pi\varepsilon}\frac{1}{|\vec{r}_e-\vec{r}_h|}. \tag{5}$$

This procedure leads to a differential equation in ρ for each carrier $[H_i-E_i]\psi_i(\rho_i)=0$, which is solved by a discretization method[25] with an uniform mesh, and the binding energy follows from $E_b=\langle\Psi|H_{e-h}|\Psi\rangle$, which yields

$$E_b=-\frac{\hbar^2}{2\mu_\perp}\int_{-\infty}^{+\infty}\phi^*(z)\frac{\partial^2}{\partial z^2}\phi(z)dz - \frac{e^2}{4\pi\varepsilon}\int_V\frac{|\psi_e(\rho_e)|^2|\psi_h(\rho_h)|^2|\phi(z)|^2}{(z^2+|\vec{\rho}_e-\vec{\rho}_h|^2)^{1/2}}dV, \tag{6}$$

where $dV=\rho_e d\rho_e\rho_h d\rho_h d\theta\, dz$ and the integral of the Coulomb term is carried out over a cylinder with an infinite interval along the z direction. Since $\phi(z)$ is a variational function such that in Eq. (2), one can solve analytically the first term integral

$$\int_{-\infty}^{+\infty}\phi^*(z)\frac{\partial^2}{\partial z^2}\phi(z)dz=-\frac{1}{\eta^2}, \tag{7}$$

and the second term assumes the form

$$-\frac{e^2}{4\pi\varepsilon\eta}\sqrt{\frac{2}{\pi}}\int_V\frac{|\psi_e(\rho_e)|^2|\psi_h(\rho_h)|^2\exp(-2z^2/\eta^2)}{(z^2+\rho_e^2+\rho_h^2-2\rho_e\rho_h\cos\theta)^{1/2}}dV, \tag{8}$$

which is simplified, leading to the final expression for the binding energy

$$E_b=\frac{\hbar^2}{2\mu_\perp\eta^2}-\frac{e^2}{4\pi\varepsilon\eta}\sqrt{\frac{2}{\pi}}\int_0^{+\infty}|\psi_e(\rho_e)|^2\rho_e \times\int_0^{+\infty}|\psi_h(\rho_h)|^2\rho_h\int_0^{2\pi}\exp(a)K_0(a/2)d\rho_e d\rho_h d\theta, \tag{9}$$

where $a=-2|\vec{\rho}_e-\vec{\rho}_h|^2/\eta$ and $K_0(x)$ is the modified zero-order Bessel function of the second kind.[26] These integrals are calculated numerically, and the exciton energy is obtained by $E_{exc}=E_{gap}+E_e+E_h-E_b$.

In type-II systems, since the potential for the electron has a step form, the electron is no more confined by the band mismatch of the wire materials, but it is just bounded by the Coulomb interaction. This implies that solving the Schrödinger equation for the electron in the absence of a Coulomb interaction leads to an electron energy $E_e=0$. To solve the type-II problem, one takes the same form of $\Psi(\rho_e,\rho_h,\theta,z)$ used previously for the type-I case in $H_{exc}|\Psi\rangle=E_x|\Psi\rangle$ and multiplies it by the complex conjugate of the ρ_h and z dependent parts of the wave function.[27] Therefore, the Schrödinger equation with the one particle Hamiltonian of Eq. (4) is solved first for the hole, so that

$$E_x|\psi_e\rangle=(H_e+E_h+\langle\psi_h\phi|H_{e\text{-}h}|\psi_h\phi\rangle)|\psi_e\rangle. \tag{10}$$

Once the hole wave function ψ_h is known, the electron effective Coulomb potential due to the presence of the hole is calculated, yielding the following differential equation for $\psi_e(\rho_e)$:

$$[H_e+E_h+I(\rho_e)]\psi_e(\rho_e)=E_x\psi_e(\rho_e), \tag{11}$$

where $I(\rho_e)=\langle\psi_h\phi|H_{e-h}|\psi_h\phi\rangle$ is the effective Coulomb potential, given by

$$I(\rho_e)=-\frac{\hbar^2}{2\mu_\perp}\int_{-\infty}^{+\infty}\phi^*(z)\frac{\partial^2}{\partial z^2}\phi(z)dz - \frac{e^2}{4\pi\varepsilon}\int_{-\infty}^{+\infty}\int_0^{2\pi}\int_0^{+\infty}\frac{|\psi_h(\rho_h)|^2|\phi(z)|^2}{(z^2+\rho_e^2+\rho_h^2-2\rho_e\rho_h\cos\theta)^{1/2}} \times\rho_h d\rho_h d\theta\, dz, \tag{12}$$

which is simplified such as in the type-I case,[26] yielding to

TABLE I. Selected properties of Si and Ge, which are used to obtain values for $Si_{1-x}Ge_x$ by linear interpolation (Ref. 8).

	a (Å)	E_g (eV)	$\epsilon(\epsilon_0)$	$m_e(m_0)$	$m_{hh}^{\perp}(m_0)$	$m_{hh}^{\parallel}$
Si	5.43	1.12	12.1	0.191	0.277	0.216
Ge	5.65	0.66	16.0	0.081	0.208	0.057

$$I(\rho_e) = \frac{\hbar^2}{2\mu_\perp \eta^2} - \frac{e^2}{4\pi\varepsilon\eta}\sqrt{\frac{2}{\pi}}\int_0^{+\infty} |\psi_h(\rho_h)|^2 \rho_h \int_0^{2\pi} \times \exp(a) K_0(a/2) d\rho_h d\theta. \quad (13)$$

The parameter η is adjusted to minimize the exciton energy E_x, as in the variational method developed for type-I wires, and now the exciton binding energy is given by $E_b = E_h - E_x$.

III. RESULTS AND DISCUSSIONS

The binding and total exciton energies in $Si/Si_{1-x}Ge_x$ QWRs are calculated for several wire radii and interface thicknesses, with $x=0.15$ (type I) and $x=0.30$ (type II). The material parameters of the alloy were obtained by an interpolation of pure Si and Ge parameters, which are listed in Table I.

A. Type-I $Si/Si_{0.85}Ge_{0.15}$ QWR

Figure 1 shows the binding energy (top) and the ground state energy (bottom) of *e-hh* excitons as a function of the $Si/Si_{0.85}Ge_{0.15}$ QWR radius (type-I band alignment) for several interface thicknesses. It can be observed that E_b increases when the wire radius increases up to a maximum at $R \sim 50$ Å, and after this it decreases. For wire radii below this value, the inclusion of a graded interface shifts down the binding energies, while the opposite occurs for a larger radii. This can be explained by considering that reducing the wire radius makes the system seem like bulk Si, where the binding energies are naturally lower.[28] For a 30 Å wire radius with interface thickness of $w=15$ Å, the binding energy is reduced by ~25%, while for wire radii greater than 50 Å there is an average increase in the binding energies of about 5.5%, in relation to the abrupt case.

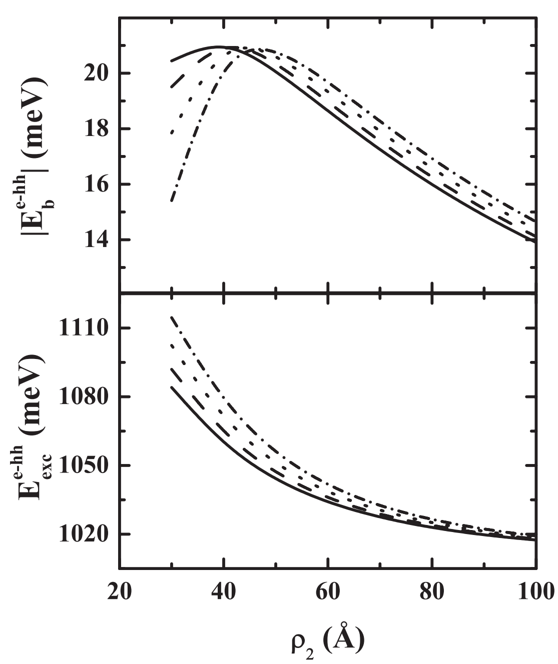

FIG. 1. Binding energy (top) and ground state energy (bottom) of *e-hh* excitons in $Si/Si_{0.85}Ge_{0.15}$ type-I QWR as a function of the wire radius, for interface thicknesses w of 0 Å (solid), 5 Å (dashed), 10 Å (dotted), and 15 Å (dashed-dotted).

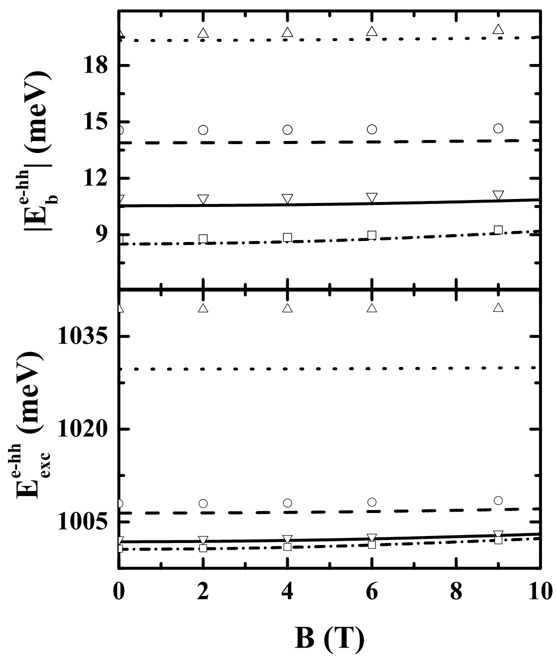

FIG. 2. Binding (top) and ground state exciton energies (bottom) of *e-hh* pairs in $Si/Si_{0.85}Ge_{0.15}$ type-I quantum wires as functions of magnetic field, with $w=0$ Å (lines) and $w=15$ Å (symbols), for several values of wire radius ρ_2: 50 Å (dotted, △), 100 Å (dashed, ○), 150 Å (solid, ▽), and 200 Å (dashed-dotted, □).

On the other hand, the ground state exciton energy always decreases with the increase of the wire radius, and the inclusion of a graded interface shifts up this energy, especially for thin wires, where these shifts may reach about 30 meV. For a 50 Å radius $Si/Si_{0.85}Ge_{0.15}$ QWR with interface thickness of $w=15$ Å, the increase in the total exciton energy is about 10 meV in relation to the abrupt case.

The influence of applied magnetic fields on the binding (top) and total (bottom) ground state exciton energies is presented in Fig. 2 for several values of the wire radius, for an abrupt interface (lines) and for a $w=15$ Å (symbols) interface thickness. As can be seen, the magnetic field does not greatly affect these energies, giving them only small blueshifts of the order of 2 meV, for all values of wire radii considered. Wires with larger radii are more affected by this external field. These results are in good agreement with previous studies in such systems for other materials.[15,29]

B. Type-II $Si/Si_{0.70}Ge_{0.30}$ QWR

Figure 3(a) shows the effective potential $V_{eff}(\rho_e) = V_e^{het}(\rho_e) + I(\rho_e)$ for electrons in type-II quantum wires. A

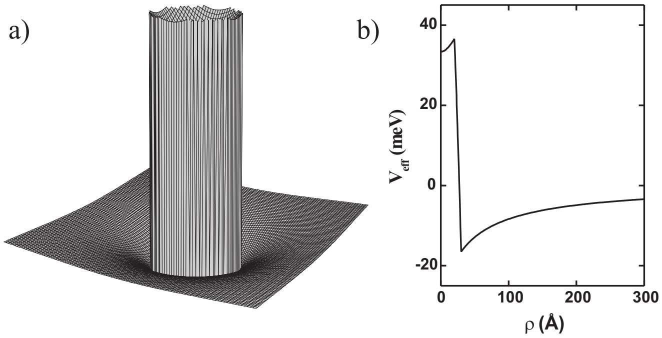

FIG. 3. (a) Effective Coulomb potential for electrons in a type-II $Si/Si_{1-x}Ge_x$ QWR with 50 Å wire radius. (b) The plot of this potential as a function of ρ, showing a depression near the interface between materials.

plot of this potential as a function of ρ is shown in Fig. 3(b), where it can be clearly seen that a depression in the potential appears due to the electron-hole Coulomb interaction, which is responsible for the electron bound state at the silicon layer near the $Si_{0.70}Ge_{0.30}$ wire, despite the fact that the heterostructure forms a barrier for this carrier.

In Fig. 4, the binding energy (top) and the ground state energy (bottom) of *e-hh* excitons are plotted as a function of the QWR radius for $Si/Si_{0.70}Ge_{0.30}$ (type-II band alignment) wires with several interface thicknesses. The binding energies of type-II wires are lower than those of type I, which is expected, since in type-II systems the electron and hole are localized in different regions of space. Moreover, these energies are always reduced when the wire radius is enlarged. This occurs because now, in the limit of very thin wires, the

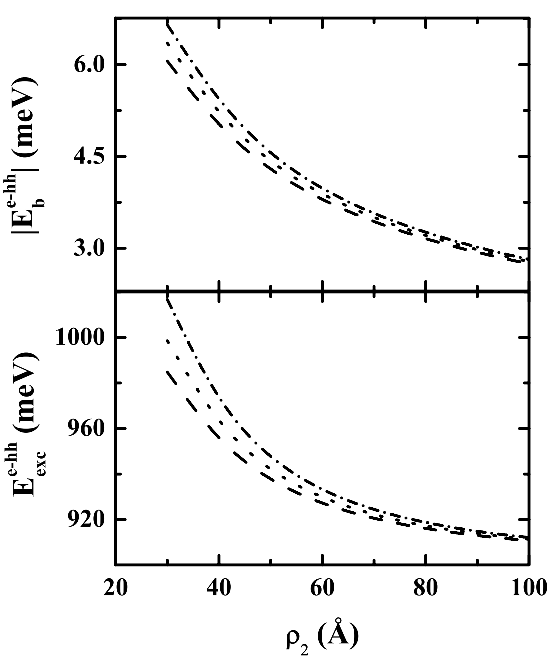

FIG. 4. Binding energy (top) and ground state energy (bottom) of *e-hh* excitons in $Si/Si_{0.70}Ge_{0.30}$ type-II QWR as a function of the wire radius, for interfaces thicknesses w of 0 Å (solid), 5 Å (dashed), 10 Å (dotted), and 15 Å (dashed-dotted).

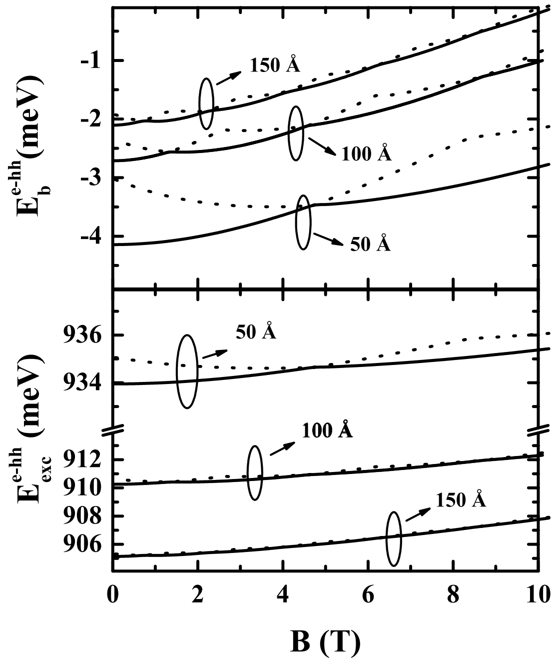

FIG. 5. Binding energies (top) and total exciton energies (bottom) of *e-hh* excitons in $Si/Si_{0.70}Ge_{0.30}$ type-II QWR as a function of the magnetic field for 50, 100, and 150 Å wire radii, with abrupt interfaces. Solid lines are related to ground state excitons, while dotted lines are first excited states.

system no more seems like bulk Si, but like a bulk system with a localized impurity, since the hole is confined within the thin wire, while the electron is bound to it on the Si layer. For a $Si/Si_{0.70}Ge_{0.30}$ with 40 Å wire radius and $w=15$ Å interface thickness, the increase of binding energies is about 12% in relation to the abrupt case, while the total exciton energy is increased by about 20 meV.

Figure 5 depicts the influence of a magnetic field parallel to the wire axis on the excitonic behavior of $Si/Si_{0.70}Ge_{0.30}$ quantum wires with abrupt interfaces for the ground and first excited states. The split between these two states is large for the thinner wire, but it is reduced as the wire radius increases, becoming very small for a 150 Å wire radius, especially for the total exciton energy (bottom). It is also shown that the binding and total exciton energies in type-II wires oscillate almost periodically as the magnetic field increases, due to changes of the angular momentum of the electrons. The periodicity of the electron angular momentum depends on the wire radius. This can be explained by the fact that only the electrons in this system are localized around the wire, which causes the magnetic field to push the electron towards the barrier, giving rise to a change in l in each electron state, because this is energetically more favorable. Since the holes are localized inside the wire, they are just squeezed towards the wire axis by the magnetic field, hence there is no change in their angular momentum. These changes in l induced by an increase of a magnetic field are analogous to the Aharonov-Bohm effect, which has been widely studied lately for several structures where carriers are localized around a barrier potential, such as quantum-rings.[30–32]

Although type-II wires have a ringlike potential for the electron, the periodicity of the Aharonov-Bohm oscillations

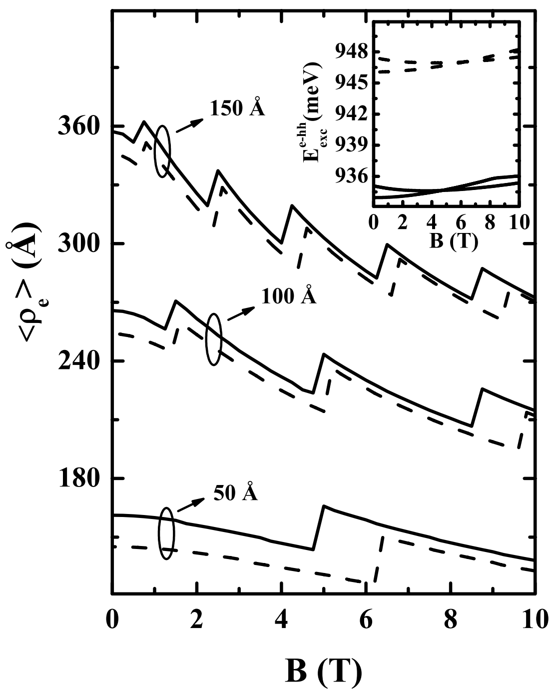

FIG. 6. Average radius of the electron ground state in $Si/Si_{0.70}Ge_{0.30}$ type-II QWR as a function of the magnetic field, for 50, 100, and 150 Å wire radii, considering $w=0$ Å (solid) and $w=15$ Å (dashed). Inset: Exciton energy dependence with the applied magnetic field, for the ground and first excited states of a 50 Å QWR radius with $w=0$ Å (solid) and $w=15$ Å (dashed).

exhibits small changes by increasing the magnetic field, in contrast to the energy states of quantum-ring structures where this periodicity is constant and well defined.[30,31,33] There is a clear dependence of the periodicity on the sectional area of the wire: the number of electron angular momentum transitions increases when the wire radius increases, representing a lower period for a larger radius. Since the periodicity depends on the area enclosed by the ringlike potential, its variation even for a constant wire radius can also be explained. In fact, increasing the magnetic field changes the hole wave function, causing the effective Coulomb potential to vary with the field, and consequently, the area enclosed by the effective potential for electrons does not remain constant for all values of the field, implying in a change of the periodicity of the AB oscillations.

The electron behavior in type-II wires under applied magnetic fields is further illustrated in Fig. 6, which shows the average radii of the electron ground state ($\langle \rho_e \rangle$) as a function of the applied magnetic field, for three values of wire radius with interface thicknesses of $w=0$ Å and $w=15$ Å. The inset shows the exciton energies related to a 50 Å QWR radius, for ground and first excited states, considering abrupt and nonabrupt interfaces. Increases of the magnetic field also give rise to oscillations in $\langle \rho_e \rangle$, which is expected since the angular momentum of this carrier is changing almost periodically, and wave functions for states with a larger modulus of angular momentum are more extensive than those for $l=0$. Thus, when the magnetic field pushes the electron towards the $Si_{1-x}Ge_x$ layer, its average radius decreases until a change of angular momentum occurs, when l assumes a higher modulus value, which implies a more spread electron wave function. For magnetic fields varying from 0 up to 10 T, for a 50 Å wire radius there is just one transition, whereas for a 150 Å wire radius there are five such transitions. It also can be seen in Fig. 6 that a graded interface affects the angular momentum transition points of AB oscillations, which is expected since the inclusion of such an interface reduces the effective radius of the quantum wire potential. Indeed, its influence on the transition points of AB oscillations can be observed even for larger radii. For a 150 Å wire radius with an abrupt interface, the fifth electron angular momentum transition occurs in a magnetic field B about 8.75 T, while for a $w=15$ Å interface it occurs at $B \simeq 9.4$ T. For a smaller radius, 50 Å, for example, this effect is stronger: the first transition occurs at $B \simeq 5$ T for an abrupt interface, whereas for $w=15$ Å it occurs at $B \simeq 6.4$ T. An exciton energy blueshift also appears due to the inclusion of graded interfaces, as one can observe in the inset of Fig. 6, which is consistent with earlier results of Fig. 4 (bottom).

IV. CONCLUSIONS

We have investigated the excitonic properties of $Si/Si_{1-x}Ge_x$ cylindrical quantum wires with type-I and type-II band alignments. Our results show that the existence of a graded interface between materials gives a significant blueshift of the exciton energies for thin wires. The presence of a magnetic field parallel to the wire axis does not greatly affect the ground state excitons in type-I QWR, especially for smaller wire radii. However, such a field alters drastically the excitonic behavior for type-II wires, since the ringlike shape of electron states is responsible for the occurrence of the Aharonov-Bohm effect, where the angular momentum l of each electron state changes almost periodically by increasing magnetic field, whereas the l of hole ground states remains the same for all B. The periodicity of these energy oscillations depends on the area enclosed by the electron effective confinement potential. This explains the nonperiodicity of Aharonov-Bohm oscillations in such systems, since the area of the effective Coulomb potential produced by the hole is altered by changes of the magnitude of the external field, which squeezes the hole wave function towards the wire axis. For a type-II $Si/Si_{0.70}Ge_{0.30}$ QWR with 40 Å wire radius, and $w=15$ Å interface thickness, the binding energies increase about 12% in relation to the abrupt case, while the total exciton energy is blueshifted by about 20 meV. Graded interfaces alter the angular momentum AB periodicity even for a larger wire radius.

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*Electronic address: jusciane@fisica.ufc.br
†Electronic address: andrey@fisica.ufc.br
‡Electronic address: king@fisica.ufc.br
§Electronic address: gil@fisica.ufc.br

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