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Excitons in quantum wires

M. Combescot[a] and T. Guillet

Groupe de Physique des Solides, CNRS, Universités Pierre et Marie Curie et Denis Diderot, 2 place Jussieu, 75251 Paris Cedex 05, France

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Abstract. This paper deals with excitons in quantum wires. We first study these excitons as the limit of excitons in D dimensions when $D \to 1$. In order to do it, we have had to find a new resolution of the hydrogen atom Schrödinger equation: besides the fact that the usual resolution found in textbooks is not valid for D exactly equal to 1, it is, surprisingly enough, inconsistent since it relies on two hypergeometric functions which are *not independent* for the parameters of physical interest! In a second part, we write down the *exact* potential felt by the exciton relative motion along the wire in terms of the wire confinement. This allows a quite precise determination of the effective Coulomb potential for this 1D motion, which is of crucial importance to obtain a meaningfull finite value for the exciton ground state energy. In a last part, we study the dependence of the exciton energies on the wire area and anisotropy. While the quantitative results are here given for cylindrical and rectangular wires with infinite barriers, we show how they can easily be extended to any particular wire shape and barrier height.

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Introduction

Nowadays, essentially all experimental and theoretical works in semiconductors physics are devoted to confined geometries. As the physics in quantum wells is now well understood, most of the efforts actually deal with quantum wires and quantum dots.

With respect to the exciton, these two types of confined structures are conceptually quite different: in quantum wires, the electrons and holes are free to move along the wire direction, so that Coulomb interaction between them plays a dominant role for the electron and the hole to stay close to each other in a bound state. On the opposite, in a quantum dot, the electrons and holes have no choice: they are forced to stay aside by the confinement potential which then acts in all three directions. When the dots are very small, this confinement produces a kinetic energy much larger than the Coulomb energy; so that, even if this Coulomb energy is *quantitatively* larger than its bulk exciton value (the electrons and holes being usually closer in a dot than the 3D Bohr radius), Coulomb interaction can be treated as a *perturbation in quantum dots* while it has to be treated *exactly for quantum wire excitons* as it is responsible for the bound states, *i.e.* for the poles in the response function which cannot be generated within finite perturbation theory. On that respect, the theory of electron-hole pairs in small quantum dots has some similarity with the theory of electron-hole drops [1] in bulk samples performed long ago. The only real difference comes from the fact that in quantum dots the quantification of the $\overrightarrow{k}$ momenta in $2\pi/L$ plays a crucial role so that the sums over $\overrightarrow{k}$ cannot be replaced by $V/(2\pi)^3$ integrals over $\overrightarrow{k}$. As a semantic consequence, even if this is now widely spread, one should not speak of excitons in quantum dots, but of electron-hole pairs, the physics induced by Coulomb interaction being usually quite easy to derive from perturbation theory at lowest order only.

The problem of excitons in quantum wires is also quite different from the problem of excitons in quantum wells [2]: indeed, while the 2D Schrödinger equation [3,4] for the electron-hole relative motion has a finite ground state energy, this is not the case for exact 1D systems. A way to intuitively grasp this point is to say that, in order to go from the left of the hole to its right, the electron of the exact 1D wire has to "pass on top of the hole" — which induces a singularity — while in a 2D quantum well, it can always go around. This intuitive argument also shows that the singularity is an artefact of the 1D limit. It is actually unphysical as real quantum wires always have a finite thickness. Consequently, the 1D singular behavior must disappear if one uses "broadened" 1D effective Coulomb potentials. It becomes then obvious that the precise *finite* value of the ground state energy, which results from the broadening, crucially depends on the way the 1D Coulomb potential is broadened. It is thus quite important to derive this broadening as correctly as possible and, if an approximate effective 1D potential has finally to be used, it is

[a] e-mail: combescot@gps.jussieu.fr

necessary to have a quantitative estimate of the uncertainty induced by this approximate potential.

The broadening of the 1D effective Coulomb potential is usually introduced by the way of a simple threshold length in the expression of the Coulomb potential, its dependences on the wire size and anisotropy being far from safely controlled [5,6]. Other works on excitons in quantum wires rely on variational [7] or fully numerical [8] procedures. These variational procedures are however known to possibly hide a large amount of the physics since they can give a good value for the ground state energy even if the variational wave functions are far from reality. Moreover they are quite dangerous for excited states as we have recently shown in the particular case of spherical quantum dots [9].

The goals of the present paper is to give an overview of what can be analytically understood on excitons in quantum wires, paying particular attention to the physical parameters of the problem, namely dimensionality, effective thickness, wire area and anisotropy.

The paper is organized as follows:

- In a first part, we reconsider the main results on excitons in 3D, 2D and 1D systems in the light of the Schrödinger equation written for S excitons in D dimensions, with D being a continuous parameter. Besides the fact that the usual procedure found in textbooks cannot be used for D strictly equal to 1, this usual procedure relies on a resolution of the Schrödinger equation which is strangely enough inconsistent: we have been amazed to realize that the general solution of the corresponding second order differential equation is given as a linear combination of two hypergeometric functions F and U which are independent *except* for the parameters of physical interest! Consequently, the first part of this paper contains a new resolution of this Schrödinger equation. For 3D and 2D, it (of course) gives the same energies and wavefunctions as the previous ones. However, relying on two solutions constructed on the hypergeometric function U only, which are defined and really independent for all values of the parameters, they can also be used for D exactly equal to 1. A special study is devoted to this 1D case, as it is the one of interest for quantum wires. We in particular derive the 1D exciton energies when the Coulomb potential has a constant broadening.

- In a second part, we determine the *exact* effective Coulomb potential induced by the confinement, felt by the 1D motion along the wire. This allows us to write down its dominant contribution for narrow wires in a secure way and also to estimate the size of the dropped terms quantitatively, in order to determine when they do give negligible contributions to the quantum wire exciton energies.

- In a third part, we calculate the exciton energies for cylindrical and rectangular wires. These geometries correspond to the two cases for which the confinement perpendicular to the wire direction generates wavefunctions which are known analytically (even for finite barriers) [14]. By writing the two lengths of the rectangular wires as $L_x = R\sqrt{\pi\ \eta}$ and $L_y = R\sqrt{\pi/\eta}$ so that the cylindrical and rectangular wires have the same area πR^2, we can easily study the dependence of the exciton energy on the wire area πR^2 as well as on the wire anisotropy $\eta = L_x/L_y$.

The quantitative results given here correspond to cylindrical and rectangular wires with infinite barriers only, as the corresponding confinement is then easy to handle analytically. Let us however stress that it is *straightforward to extend the present calculations to any wire shapes and barrier potentials*: one just has to determine the values of the three parameters $a_{11} = (a_{1,1;11})$, $b_{11} = (b_{1,1;11})$ and $c_{11} = (c_{1,1;11})$ defined in equations (2.15, 2.16), which characterize the 1D effective Coulomb potential appropriate to the wire confinement of interest, and to solve numerically the 1D Schrödinger equation (2.17) corresponding to the effective potential $b_{11}(z)$ given in equation (2.18).

1 Exciton Schrödinger equation in D dimension

From the radial part of the Laplacian in $D = d + 1$ dimensions, we get the Schrödinger equation for the relative motion of S excitons as:

$$\left(-\frac{\hbar^2}{2\mu}\frac{1}{r^d}\frac{\partial}{\partial r}\left(r^d\frac{\partial}{\partial r}\right) - \frac{e^2}{r}\right)\psi_E^{(d)}(r) = E\psi_E^{(d)}(r) \quad (1.1)$$

with $\mu^{-1} = m_e^{-1} + m_h^{-1}$. The d's of physical interest are of course $d = (2, 1, 0)$. By using the Landau rescaling [12]

$$E = -R_X/\lambda^2\ ; \quad r = \lambda\rho a_X/2 \quad (1.2)$$

with $R_X = \hbar^2/(2\mu a_X^2) = e^2/(2a_X)$, this Schrödinger equation for $\psi_E^{(d)}(r)$ transforms into a Schrödinger equation for $\varphi_{\lambda,d}(\rho) = \psi^{(d)}_{-R_X/\lambda^2}(\lambda\rho a_X/2)$, which reads

$$\varphi''_{\lambda,d} + \frac{d}{\rho}\varphi'_{\lambda,d} + \left(\frac{\lambda}{\rho} - \frac{1}{4}\right)\varphi_{\lambda,d} = 0. \quad (1.3)$$

Bound states correspond to $\lambda^2 > 0$, *i.e.* λ real, while extended states correspond to λ imaginary. As $+\lambda$ and $-\lambda$ give the same energy, we will choose to call λ either $(+\sqrt{\lambda^2})$ if $\lambda^2 > 0$ or $(+\mathrm{i}\sqrt{-\lambda^2})$ if $\lambda^2 < 0$, the intrinsic $(\pm\lambda)$ symmetry of the problem having *a priori* to appear in a natural way in the general solutions of the Schrödinger equation. We will come back to this important point later on.

Equation (1.3) can be solved analytically in terms of hypergeometric functions. We will first give the usual procedure found in textbooks [12]. However, this procedure is utterly weak as it relies on a "general" solution of the second order differential equation (1.3) made out of two solutions which are, surprisingly enough, exactly proportional for the λ's of physical interest. As in addition, this usual procedure does not hold for 1D system (which is the interesting case for quantum wires), in a second paragraph, we will give another procedure valid for all dimensions and which allows to write down two really independent solutions for any values of the parameters λ and d.

1.1 Usual resolution of the Schrödinger equation

By considering the large ρ limit of equation (1.3), namely $\varphi''_{\lambda,d} - \varphi_{\lambda,d}/4 = 0$, the solutions of which are $e^{\pm\rho/2}$, we are led to set, following Landau-Lifschitz [12]:

$$\varphi_{\lambda,d}(\rho) = e^{-\rho/2} g_{\lambda,d}(\rho). \tag{1.4}$$

Even if this may appear a nice idea at first as it extracts one of the two possible asymptotic behaviors of $\varphi_{\lambda,d}(\rho)$, we note that equation (1.4) obviously destroys the initial $(\lambda,\rho) \leftrightarrow (-\lambda,-\rho)$ symmetry of the rescaling done in equation (1.2), which is clearly a weak point for this procedure.

By inserting equation (1.4) into equation (1.3), we find that $g_{\lambda,d}(\rho)$ verifies the differential equation for degenerate hypergeometric functions, namely

$$z f'' + (c - z) f' - a f = 0 \tag{1.5}$$

with $a = d/2 - \lambda$ and $c = d$.

For "non-pathological" values of the parameters a and c, the two independent solutions of this equation (1.5) are said to be [10] $F(a,c,z)$ and $z^{1-c}F(a-c+1,2-c,z)$ where $F(a,c,z)$ is defined by the serie

$$F(a,c,z) = 1 + \frac{a}{c}\frac{z}{1!} + \frac{a(a+1)}{c(c+1)}\frac{z^2}{2!} + ... \tag{1.6}$$

(This can be easily checked by inserting Eq. (1.6) into Eq. (1.5).)

One pathological value of the parameter c is obviously $c = 1$ as the two solutions are then identical. Other pathological values of c are $c = (0,-1,-2,...)$ since $F(a,c,z)$ has no meaning for such c's. In a similar way, $F(a-c+1,2-c,z)$ is meaningless for $c = 2,3,....$ We thus conclude that $F(a,c,z)$ and $z^{1-c}F(a-c+1,2-c,z)$ cannot be used as the two independent solutions of equation (1.5) if c is an integer. As the c's of physical interest for the exciton problem are $c = d = D-1$, these two solutions can be used neither for 1D ($d = 0$) nor for 2D or 3D ($d = 1$ or 2) systems.

Following Abramowitz and Stegun, we can think to another couple of solutions for this equation (1.5), namely $F(a,c,z)$ and $U(a,c,z)$ with U defined as [11]

$$U(a,c,z) = \frac{\pi}{\sin\pi c}\left(\frac{F(a,c,z)}{\Gamma(c)\Gamma(1+a-c)} - c z^{1-c}\frac{F(a+1-c,2-c,z)}{\Gamma(2-c)\Gamma(a)}\right). \tag{1.7}$$

In view of the above definition of U, it may appear as reasonable to believe that $F(a,c,z)$ and $U(a,c,z)$ are indeed two independent functions. More surprising can be the fact that this function $U(a,c,z)$ is defined for any values of the parameters, in particular even for integer c's [11]. This is however transparent from the serie expansion of U given by [13]

$$U(a,c,z) = z^{-a} G(a,a+1-c,-z) \tag{1.8}$$

$$G(a,\gamma,z) = 1 + \frac{a\gamma}{1!z} + \frac{a(a+1)\gamma(\gamma+1)}{2!z^2} + ... \tag{1.9}$$

Although not widely used, this serie expansion of $U(a,c,z)$ is quite convenient for analytical purposes. From it, it is easy to check that such a $U(a,c,z)$ is indeed solution of equation (1.5). It is also easy to check that

$$U'(a,c,z) = -aU(a+1,c+1,z). \tag{1.10}$$

Being (apparently) independent of $F(a,c,z)$ and defined for all c's, the function $U(a,c,z)$ can advantageously replace $z^{1-c}F(a-c+1,2-c,z)$ as a second solution of equation (1.5). Consequently, it is usually claimed that the general solution of equation (1.3) writes

$$\varphi_{\lambda,d}(\rho) = e^{-\rho/2}\left[A\ F(d/2-\lambda,d,\rho) + B\ U(d/2-\lambda,d,\rho)\right] \tag{1.11}$$

with still an exception for 1D systems as $F(d/2-\lambda,d,\rho)$ is meaningless for $d = 0$.

The parameters A and B are determined by enforcing two boundary conditions:

(i) The wave function must stay finite when $\rho \to 0$. This lead to $B = 0$ as $U(d/2-\lambda,d,\rho \to 0)$ is said to diverge for $c \geq 1$: indeed, reference [11] gives

$$\begin{aligned} U(a,c,\rho\to 0) &\simeq \frac{\Gamma(c-1)}{\Gamma(a)}\rho^{1-c} \quad \text{if } c > 1 \\ &\simeq \frac{1}{\Gamma(a)}\ln(1/\rho) \quad \text{if } c = 1 \\ &\simeq \frac{\Gamma(1-c)}{\Gamma(1+a-c)} \quad \text{if } c < 1. \end{aligned} \tag{1.12}$$

(ii) For bound states, the wave function has to go to zero when $\rho \to \infty$. As $F(a,c,\rho\to\infty)$ is said to diverge as $\exp(\rho)$, we would get $A = 0$, *i.e.* $\varphi_{\lambda,d}(\rho) \equiv 0$ which would be dramatic. However $F(a,c,\rho\to\infty)$ behaves as $\exp(\rho)$ except if F is a finite serie, *i.e.* if $a = d/2-\lambda = -n$ with $n = 0,1,2...$ Consequently, the λ's for bound states must be equal to $n+d/2$, the corresponding energies being given by

$$E_{n,d} = -\frac{R_X}{(n+d/2)^2}, \qquad n = (0,1,2...) \tag{1.13}$$

with $d = 2$ for 3D excitons and $d = 1$ for 2D excitons.

Although the above energies are fully correct (of course), the way they have been reached is not: indeed the reason to eliminate the solution with U is (surprisingly enough) incorrect as $U(a,c,z)$ diverges for $\rho \to 0$ except for $a = 0,-1,-2,...$, which are exactly the a's of interest, as the asymptotic serie given in equations (1.8, 1.9) is then finite. This can also be seen from the small z behavior of $U(a,c,z)$ as $\Gamma(a)$ diverges for $a = 0,-1,-2,....$ For such a's, the functions F and U are in fact proportional! Using equations (1.6, 1.8, 1.9), it is easy to check that

$$U(-n,c,z) = (-1)^n c(c+1)...(c+n-1)F(-n,c,z) \tag{1.14}$$

with $U(0,c,z) = F(0,c,z) = 1$. Consequently, for the λ values of physical interest, the two *independent* solutions of equation (1.3) cannot be $e^{-\rho/2}F(d/2-\lambda,d,\rho)$ and $e^{-\rho/2}U(d/2-\lambda,d,\rho)$ as usually claimed.

Since, in addition, the solution with F is meaningless for $d = 0$, *i.e.* for 1D excitons, it is necessary to find another procedure to determine the two really *independent* solutions of equation (1.3) valid for any values of the parameters. This new procedure will fully use the intrinsic $(\pm\lambda)$ symmetry of the problem missed by the usual procedure.

1.2 New resolution of the Schrödinger equation valid for any values of the space dimension and the energy

From the above discussion, we have identified one possible solution of equation (1.3) valid for any values of λ and d, namely

$$\begin{aligned}\Phi_{\lambda,d}(\rho) &= \mathrm{e}^{-\rho/2} U(d/2-\lambda, d, \rho) \\ &= \mathrm{e}^{-\rho/2}\ \rho^{\lambda-d/2}\ \left[1 - \frac{(d/2-\lambda)(1-d/2-\lambda)}{1!\ \rho}\right. \\ &\left. + \frac{(d/2-\lambda)(1+d/2-\lambda)(1-d/2-\lambda)(2-d/2-\lambda)}{2!\ \rho^2} - ...\right]\end{aligned} \tag{1.15}$$

(It is straightforward to check that this $\Phi_{\lambda,d}(\rho)$ is indeed solution of Eq. (1.3) by inserting the above expansion directly into Eq. (1.3).) If we now go back to equation (1.3), we see that, if $\Phi_{\lambda,d}(\rho)$ is a solution, $\Phi_{-\lambda,d}(-\rho)$ must also be a solution. As $U(a,c,\rho\to\infty) \approx \rho^{-a}$, the functions $\Phi_{\lambda,d}(\rho)$ and $\Phi_{-\lambda,d}(-\rho)$ are really independent for *any* (λ, d) since the first one goes to zero as $\mathrm{e}^{-\rho/2}\rho^{\lambda-d/2}$ in the large ρ limit while the other one diverges as $\mathrm{e}^{\rho/2}\rho^{-\lambda-d/2}$. Consequently the two solutions of equation (1.3) which are perfectly defined *and* really independent for *any* (λ, d), are $\Phi_{\lambda,d}(\rho)$ and $\Phi_{-\lambda,d}(-\rho)$, not $\mathrm{e}^{-\rho/2}F(d/2-\lambda,d,\rho)$ and $\Phi_{\lambda,d}(\rho)$ as widely spread.

The general solution for equation (1.3) has thus to be taken as

$$\varphi_{\lambda,d}(\rho) = A\ \Phi_{\lambda,d}(\rho) + B\ \Phi_{-\lambda,d}(-\rho). \tag{1.16}$$

For bound states, we must have $\varphi_{\lambda,d}(\rho\to\infty) = 0$, so that $B = 0$. If we also want $\varphi_{\lambda,d}(\rho)$ to stay finite for $\rho \to 0$, we must have $d/2 - \lambda = -n$ with $n = 0, 1, 2...$, in order for the serie expansion (1.15) to be finite. From these λ's, we recover the energies given in equation (1.13) of course! Although less obvious at first glance as the wave functions in equation (1.15) appear in terms of U and not in terms of F, we also recover the well known 3D and 2D exciton wave functions. Indeed, due to equation (1.14), these two functions F and U are exactly proportional for $d/2 - \lambda = -n$. This can also be directly checked for the lowest values of n by using the serie expansions of F and U given in equation (1.6) and equations (1.8, 1.9).

Although the usual definition (Eq. (1.7)) of the degenerate hypergeometric function $U(a,c,z)$ makes it much more frightening than the function $F(a,c,z)$ at first, U is safer than F as it does not suffer from constrains on the parameter c. Moreover, its serie expansion given in equations (1.8, 1.9) makes it quite similar to handle analytically as $F(a,c,z)$, so that, after all, $U(a,c,z)$ is not worse than $F(a,c,z)$!

1.3 Exact 1D case

From equation (1.13), we see that the energy of the exciton ground state ($n = 0$) should go to $-\infty$ when $d = D - 1$ goes to zero, while the energies of the excited states ($n = 1, 2, ...$) go to $-R_X/n^2$ in this exact 1D limit. The pathology of the 1D ground state exciton can also be seen from the Schrödinger equation equation (1.3): in the $\rho \to 0$ limit, this equation reads $d\varphi'_\lambda + \lambda\varphi_\lambda = 0$; so that for $d = 0$, we must have either $\varphi_\lambda(0) = 0$ if λ is finite, or $\lambda = 0$ if $\varphi_\lambda(0)$ is finite. We must however stress that the Landau rescaling done in equation (1.2), and leading to this equation (1.3), is meaningless for $\lambda = 0$; consequently, any conclusion using it and reached for λ exactly equal to 0 is *a priori* doubtful.

In the exact 1D case, the exciton problem is indeed highly pathological and difficult to study cleanly. Let us reconsider it from the beginning. 1D excitons are characterized by a relative motion wavefunction $\psi_E(z)$ with $-\infty < z < \infty$. The Coulomb energy being $(-e^2/|z|)$, the 1D exciton Schrödinger equation reads

$$-\frac{\hbar^2}{2\mu}\ \psi''_E(z) - \frac{e^2}{|z|}\ \psi_E(z) = E\ \psi_E(z).$$

It is clear that a solution corresponding to $E = -\infty$ cannot be handled cleanly from this equation: It is only possible to study the ground state quantum wire exciton as a limit. The previous paragraph allowed to reach this ground state as the limit when the space dimension D goes to 1. The next paragraph will allow to study the ground state exciton from the 1D broadened case, as the limit when the broadening goes to zero.

Even if we eliminate the ground state, the exact 1D case is still highly pathological as we now show. For finite E, the Landau rescaling $E = -R_X/\lambda^2$ and $z = \lambda\zeta a_X/2$ can be performed without ambiguity since λ will differ from 0. We then get that $\varphi_{\lambda,0}(\zeta) = \psi_{-R_X/\lambda^2}(\lambda\ \zeta\ a_X/2)$ verifies

$$\varphi''_{\lambda,0} + \left(\frac{\lambda}{|\zeta|} - \frac{1}{4}\right)\varphi_{\lambda,0} = 0. \tag{1.17}$$

The potential being an even function of ζ, the solutions of this equation are even or odd, $\varphi_{\lambda,0}(\zeta) = \pm\varphi_{\lambda,0}(-\zeta)$ while, following equation (1.16), they must read

$$\varphi_{\lambda,0}(\zeta) = A\ \Phi_{\lambda,0}(\zeta) + B\ \Phi_{-\lambda,0}(-\zeta) \tag{1.18}$$

with $\Phi_{\lambda,0}(\zeta)$ given in equation (1.15). By enforcing $\varphi_{\lambda,0}(\zeta\to\infty) = 0$, we are left with

$$\begin{aligned}\varphi_{\lambda,0}(\zeta>0) &= \Phi_{\lambda,0}(\zeta) \\ &= \mathrm{e}^{-\zeta/2} U(-\lambda, 0, \zeta) \\ &= \mathrm{e}^{-\zeta/2}\ \zeta^{\lambda}\ \left[1 - \frac{(-\lambda)(1-\lambda)}{1!\ \zeta}\right. \\ &\left. + \frac{(-\lambda)(1-\lambda)(1-\lambda)(2-\lambda)}{2!\ \zeta^2} - ...\right].\end{aligned} \tag{1.19}$$

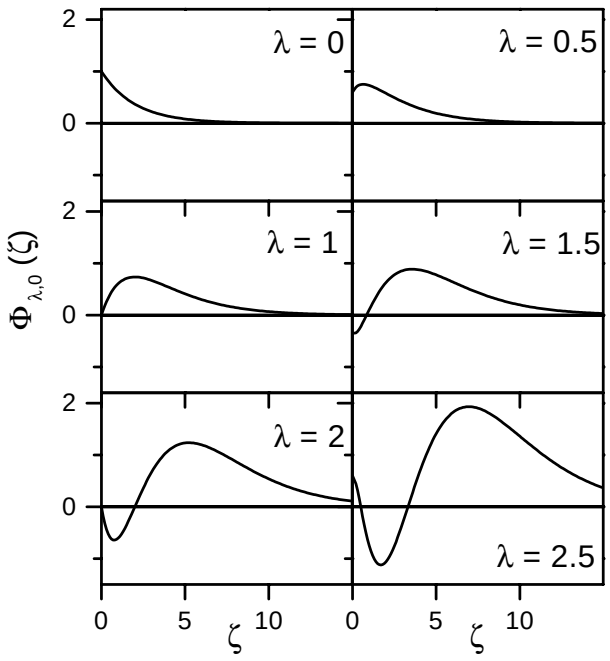

Fig. 1. ζ dependence of the function $\Phi_{\lambda,0}(\zeta) = e^{-\zeta/2}U(-\lambda,0,\zeta)$, as defined in equation (1.19), for $0<\zeta<15$ and various values of λ $(0, 0.5, 1, 1.5, 2, 2.5)$. Among these values of λ, we see that $\Phi_{\lambda,0}(0)=0$ for $\lambda=(1,2)$ only.

The functions $\Phi_{\lambda,0}(\zeta)$ for some values of λ are shown in Figure 1.

In order for $\varphi''_{\lambda,0}$ to be defined (*i.e.* finite) at the origin, odd functions must be such that $\varphi_{\lambda,0}(0)=0$ while even functions must be such that $\varphi'_{\lambda,0}(0)=0$. However, as the potential diverges for $\zeta\to 0$, equation (1.17) imposes in addition $\varphi_{\lambda,0}(0)=0$ in order for $\varphi''_{\lambda,0}(0)$ to be finite. As

$$\varphi_{\lambda,0}(\zeta\to 0) = U(-\lambda,0,\zeta\to 0) = \frac{1}{\Gamma(1-\lambda)} = \frac{\Gamma(\lambda)}{\pi}\sin\pi\lambda$$

due to equation (1.12) while $\Gamma(n+1)=n!$, we thus find that $\varphi_{\lambda,0}(0)=0$ for $\lambda=(1,2,3,...)$. This can also be seen from the serie expansion (1.19).

Consequently, we find that the possible wavefunctions of the two lowest finite energy 1D excitons are $\varphi_{1,0}(\zeta>0)=\zeta\, e^{-\zeta/2}$ and $\varphi_{2,0}(\zeta>0)=(\zeta^2-2\zeta)\, e^{-\zeta/2}$, according to equation (1.19). They are shown in Figure 2. We see that they have finite slope at the origin, so that they cannot be used to build even wavefunctions: their derivatives would have a jump for $\zeta\to 0^{\pm}$, so that $\varphi''_{\lambda,0}$ would not be defined at the origin. Let us stress that, if we accept $\varphi''_{\lambda,0}(\zeta\to 0)$ possibly infinite, there is no more reason to impose $\varphi_{\lambda,0}(\zeta\to 0^+)=0$, *i.e.* no reason to restrict the λ's to be equal to $(1,2,3,...)$.

In the next paragraph, we will show that, in the limit of a zero broadening, 1D excitons with even wavefunctions and finite $\varphi''_{\lambda,0}$ at the origin do in fact exist for $\lambda=(1,2,3,...)$. There is however no way to cleanly derive the eigenenergies of these even states from the study of the exact 1D case: it is indeed too pathological.

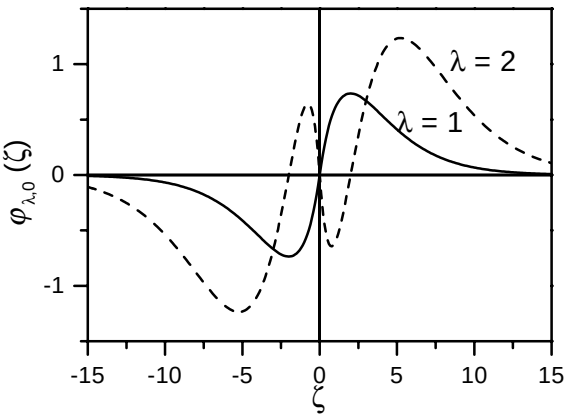

Fig. 2. Possible wave functions $\varphi_{\lambda,0}(\zeta)$ for exact 1D excitons as enforced by convergence for $\zeta\to\pm\infty$ and continuities of $\varphi_{\lambda,0}$ and $\varphi'_{\lambda,0}$ for $\zeta\to 0$: plain line $\lambda=1$, dashed line $\lambda=2$. The study of the exact 1D case leads to odd states only.

1.4 Broadened-1D excitons

In the preceding paragraph, we have shown that in the exact-1D limit, all "reasonable" solutions of the Schrödinger equation appear to be odd functions only. This pathology is again directly linked to the exact-1D limit: it is in fact spurious.

As shown in more details below, the finite thickness of the quantum wire broadens the Coulomb potential in such a way that, instead of $e^2/|z|$, it appears as

$$V_{eff}(z) = -\frac{e^2}{|z|+b(|z|)} \tag{1.20}$$

with $b(z)$ decreasing from $b(0)\neq 0$ to 0 when z increases from 0 to ∞. If we replace $b(z)$ by a constant b^* (somewhat smaller than $b(0)$ in order to optimize the fit with this effective potential) [4–6], the corresponding 1D Schrödinger equation just appears as equation (1.17) with $\lambda/|\zeta|$ replaced by $\lambda/(|\zeta|+\beta^*_\lambda)$ with

$$b^* = \lambda\ \beta^*_\lambda\ a_X/2. \tag{1.21}$$

It precisely reads

$$\hat\varphi''_{\lambda,0} + \left(\frac{\lambda}{|\zeta|+\beta^*_\lambda} - \frac{1}{4}\right)\ \hat\varphi_{\lambda,0} = 0. \tag{1.22}$$

The potential still being an even function of ζ, the general solutions of equation (1.22) are such that

$$\hat\varphi_{\lambda,0}(\zeta>0) = A\Phi_{\lambda,0}(\zeta+\beta^*_\lambda) + B\Phi_{-\lambda,0}(-\zeta-\beta^*_\lambda) = \pm\hat\varphi_{\lambda,0}(-\zeta) \tag{1.23}$$

with $\Phi_{\lambda,0}(\zeta)$ again given by equation (1.15). For bound states, $\hat\varphi_{\lambda,0}(\zeta\to\infty)=0$ imposes $B=0$ while we must have

$$\hat\varphi_{\lambda,0}(0) = 0 = \Phi_{\lambda,0}(\beta^*_\lambda) \text{ for odd solutions}$$
$$\hat\varphi'_{\lambda,0}(0) = 0 = \Phi'_{\lambda,0}(\beta^*_\lambda) \text{ for even solutions.} \tag{1.24}$$

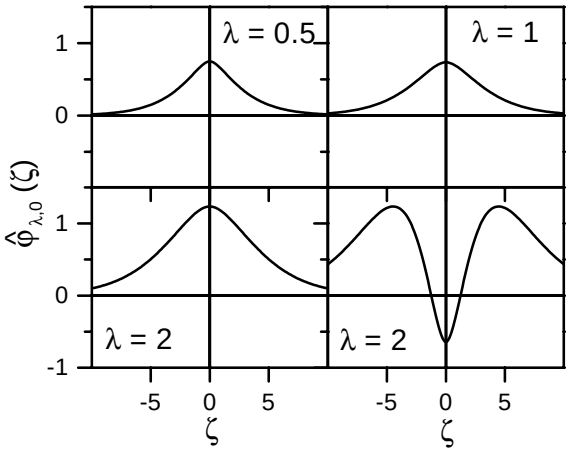

Fig. 3. Wave functions $\hat{\varphi}_{\lambda,0}(\zeta)$ for broadened-1D excitons with a constant broadening $b^* = (0.16, 1, 3 \pm \sqrt{5})$ in Bohr units a_X. ζ varies from -10 to 10. The corresponding energy parameters are $\lambda = 0.5$ for $b^* = 0.16\ a_X$, $\lambda = 1$ for $b^* = a_X$ and $\lambda = 2$ for both $b^* = (3 \pm \sqrt{5})\ a_X$. The wave functions for $b^* = (0.16, 1, 3 + \sqrt{5})$ have no node, so that they correspond to exciton ground states, while the one for $(3 - \sqrt{5})$ has one node for positive ζ so that it corresponds to an exciton first (even) excited states. Let us however stress that the ground state obtained for $b^* = (3+\sqrt{5})$, with an energy $-R_X/4$ well above bulk value, is surely meaningless: the constant broadening approximation cannot be extended up to a so large broadening.

Let us stress that, as the potential stays finite when $\zeta \to 0$, it is no more necessary to have $\hat{\varphi}_{\lambda,0}(0) = 0$ in order for $\hat{\varphi}'_{\lambda,0}$ to stay finite at the origin. This allows the existence of even wave functions as we now show.

Although the physics is to determine the exciton energies, *i.e.* the possible λ's, for a given broadening b^*, the mathematical resolution of the transcendental equations $\Phi_{\lambda,0}(\beta^*_\lambda) = 0$ or $\Phi'_{\lambda,0}(\beta^*_\lambda) = 0$ turns out to be much simpler if we look for the β^*_λ's, *i.e.* the b^*'s, which correspond to a given λ. We will first consider integer values of λ for simplicity as the $\Phi_{\lambda,0}(\zeta)$'s have then simple analytical expressions.

(i) For $\lambda = 1$, we find

$$\Phi_{1,0}(\zeta) = \zeta \mathrm{e}^{-\zeta/2} \tag{1.25}$$

as deduced from equation (1.15). $\Phi_{1,0}(\zeta)$ has one zero for $\zeta = 0$ and one extremum for $\zeta = 2$. Consequently $\lambda = 1$ is a possible energy parameter for odd functions when $\beta^*_1 = 0 = b^*$ (as already found in the preceding paragraph). It is also a possible energy parameter for even functions when $\beta^*_1 = 2$, *i.e.* $b^* = a_X$ due to equation (1.21). Consequently, for a constant Coulomb broadening equal to the 3D Bohr radius a_X, the 1D Schrödinger equation has an even solution with an energy $-R_X$. The corresponding wave function, shown in Figure 3, having no node, this state is thus the exciton ground state for the broadening $b^* = a_X$.

(ii) For $\lambda = 2$, we find

$$\Phi_{2,0}(\zeta) = \zeta(\zeta - 2)\mathrm{e}^{-\zeta/2} \tag{1.26}$$

as deduced from equation (1.15). $\Phi_{2,0}(\zeta)$ has two zeros for $\zeta = (0, 2)$ and two extrema for $\zeta = 3 \pm \sqrt{5}$. Consequently, $\lambda = 2$ is a possible energy parameter for odd states when $\beta^*_2 = 0 = b^*$ (as already shown in the preceding paragraph) and when $\beta^*_2 = 2$, *i.e.* $b^* = 2a_X$. It is also a possible energy parameter of even states when $\beta^*_2 = 3 \pm \sqrt{5} = b^*/a_X$. The wave functions for these two possible couples of solutions ($b^* = (3-\sqrt{5})a_X \approx 0.7a_X,\ \lambda = 2$) and ($b^* = (3 + \sqrt{5})a_X \approx 5a_X,\ \lambda = 2$) are shown in Figure 3. The one corresponding to the smallest b^* has one node for positive ζ so that it corresponds to an exciton (even) first excited state. The other solution could be an exciton ground state as it has no node. However, it is physically meaningless, as the constant broadening approximation for the 1D Coulomb potential is surely not valid for such a large b^*. Indeed for very wide quantum wires, the ground state exciton energy should tend to the bulk value $-R_X$, while for $b^* \approx 5a_X$, we here find that the energy would be $-R_X/4$.

(iii) For $0 < \lambda < 1$,

numerical calculations show that $\Phi_{\lambda,0}(\zeta)$ has no zero so that there is no odd solution for $\lambda < 1$, *i.e.* for energy smaller than $-R_X$. We also find that $\Phi_{\lambda,0}(\zeta)$ has one maximum only which moves from $\zeta = 0$ to $\zeta = 2$ when λ increases from 0 to 1. Figure 1 shows that, for $\lambda = 0.5$, this maximum corresponds to $\zeta \approx 0.62$. Following equation (1.21), we get the broadening corresponding to this $\beta^*_{0.5} \approx 0.62$ as being $b^* \approx 0.16a_X$. Figure 3 shows the wave function for this couple (λ, b^*). It has no node so that it corresponds to a ground state. We thus conclude that the ground state exciton energy for a constant Coulomb broadening $b^* \approx 0.16a_X$ is $-R_X/(0.5)^2 = -4R_X$. By comparing the wave functions for $b^* = 0.16\ a_X$ and $b^* = a_X$, we also see that the wave function spatial extension decreases when b^* decreases as physically expected. Following the same procedure, we can determine the broadenings for all ground states with energy parameter between 0 and 1, *i.e.* the ground state energies for all broadenings b^* between 0 and a_X. They are shown in Figure 4. We see that when $b^* \to 0$, λ goes to zero, *i.e.* the ground state energy diverges as expected. We also see that the energy do not tend to its bulk value $-R_X$ when b^* increases: this is due to the fact that the constant broadening approximation is not valid for wide quantum wires.

(iv) For $1 < \lambda < 2$,

numerical calculations show that $\Phi_{\lambda,0}(\zeta)$ has one zero which moves from $\zeta = 0$ to $\zeta = 2$ when λ increases form 1 to 2. This zero corresponds to possible odd states with broadenings between 0 and 2 a_X. The associated wave functions $\hat{\varphi}_{\lambda,0}(\zeta)$ having one node (for $\zeta = 0$), the corresponding states are exciton (odd) first excited states. For these λ's, $\Phi_{\lambda,0}(\zeta)$ has also one minimum and one maximum, so that for the same energy parameter, it also exists even states. The maxima of $\Phi_{\lambda,0}(\zeta)$ correspond to quite large values of b^* outside the range of validity of the constant broadening approximation so that we will not consider them. As for the minima, we see in Figure 1 that, when $\lambda = 1.5$, $\Phi_{\lambda,0}(\zeta)$ is minimum for $\zeta \approx 0.14$. Equation (1.21) gives the broadening associated to this

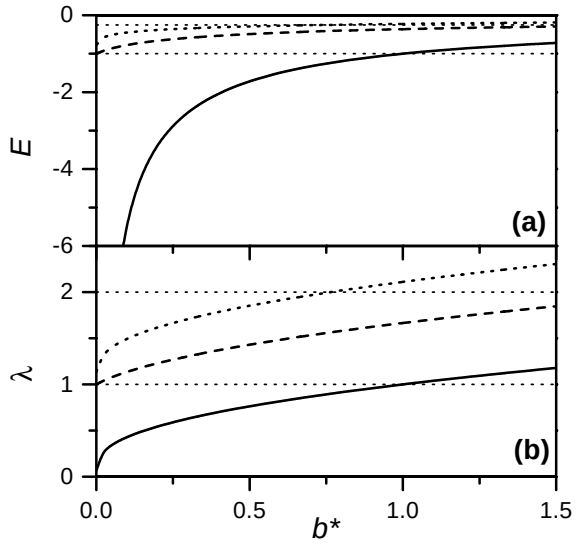

Fig. 4. (a) Energies of the exciton lowest even state (solid lines) and odd states (dashed lines), in Rydberg unit R_X, as a function of the constant Coulomb broadening parameter b^*, in a_X unit. The horizontal dotted lines correspond to the bulk energy values $-R_X$ and $-R_X/4$. (b) Energy parameters λ, as a function of b^*. The bulk values (horizontal dotted lines) correspond to $\lambda = 1$ and $\lambda = 2$. We see that the bulk values are obviously not the large b^* limit of these curves. This is due to the fact that a constant broadening for the Coulomb potential is a meaningfull approximation for small b^* only.

$\beta^*_{1.5} \approx 0.14$ as being $b^* \approx 0.11 a_X$. The corresponding wave function having one node, $\lambda = 1.5$ is thus the energy parameter of the exciton (even) first excited state when the constant broadening is $b^* \approx 0.11 a_X$.

The energies and λ parameters of the exciton quantum wire first excited states as a function of b^* are shown in Figure 4. Since, for $\lambda < 1$, the $\Phi_{\lambda,0}(\zeta)$'s have no zero and one maximum only, the λ's of these exciton first excited states are all larger than 1. The corresponding energies are thus all above $-R_X$, which appears as the limit of the first excited state energies when the the broadening goes to zero: this is in full agreement with the energy of the $n = 1$ state given in equation (1.13) when d goes to 0, *i.e.* when the space dimension D goes to 1. We also see that both odd and even states do exist when the broadening b^* goes to zero, their energy parameter λ going to 1: starting from the even wave function shown in Figure 3 for $\lambda = 2$, we find that the two zeros of this wave function move towards $\zeta = 0$ when b^* decreases from $(3 - \sqrt{5})a_X$ while λ goes to 1. This clearly shows that in the $b^* \to 0$ limit, even wave functions do exist with energy parameters λ going to 1_+: they have a cusp for $\zeta = 0$, *i.e.* an infinite second derivative at the origin; the previous paragraph on the exact 1D case did not allow us to reach such a conclusion in a clean way. Finally Figure 4 again shows that the energies obtained for large b^* are meaningless since they are above the bulk value $(-R_X/4)$.

(v) For $\lambda \to 0^+$,
the ground state energy diverges. As seen from Figure 1, this happens when the constant broadening b^* goes to zero. Here again, we recover the infinite limit of the $(n = 0)$ ground state energy as given in equation (1.13) when $d \to 0$, *i.e.* when the space dimension D goes to 1. In the last part of this Section 1, we are going to analytically study the quantum wire exciton ground state energy in this small b^* limit.

We first note that, as b^* and λ are both small in this limit, it is not *a priori* obvious that β^*_λ defined in equation (1.21) is indeed small. Let us look at this point first. Using equation (1.15), the transcendental equation $\Phi'_{\lambda,0}(\beta^*_\lambda) = 0$ also reads

$$U(-\lambda, 0, \beta^*_\lambda) = 2U'(-\lambda, 0, \beta^*_\lambda). \tag{1.27}$$

By using equation (1.10), this equation is nothing but

$$U(-\lambda, 0, \beta^*_\lambda) = 2\lambda\, U(1-\lambda, 1, \beta^*_\lambda). \tag{1.28}$$

If β^*_λ were large, equations (1.8, 1.9) would lead to

$$(\beta^*_\lambda)^\lambda \approx 2\lambda(\beta^*_\lambda)^{\lambda-1} \tag{1.29}$$

i.e. $\beta^*_\lambda \approx \lambda$ which is inconsistent with β^*_λ large while λ is small. Consequently β^*_λ is indeed small for small λ's. Using the small ζ limit of $U(a, c, \zeta)$ given in equation (1.12), equation (1.28) then gives

$$\frac{1}{\Gamma(1-\lambda)} \approx 2\lambda \frac{1}{\Gamma(1-\lambda)} \ln \frac{1}{\beta^*_\lambda},$$

so that the ground state energy parameter λ for a small constant broadening verifies:

$$\lambda e^{-1/2\lambda} \approx 2b^*/a_X \tag{1.30}$$

in agreement with reference [4]. Here again, this transcendental equation gives the broadening b^* for a given small λ much more easily than it gives the energy for a given broadening b^*.

2 Effective potential for the exciton relative motion along the wire

As shown above, the existence of a finite value for the exciton ground state energy is crucially linked to the fact that a physical quantum wire has a finite thickness which broadens the Coulomb potential acting on the z variable along the wire. In this paragraph, we are going to write the *exact* potential felt by the exciton relative motion along the wire. From it, we will extract its leading term for narrow wires and we will estimate the dropped terms.

If we forget the center of mass motion along the wire, the Hamiltonian for quantum wire excitons reads

$$H = h_e + h_h + \frac{P_z^2}{2\mu} - \frac{e^2}{\sqrt{z^2 + (\vec{\rho_e} - \vec{\rho_h})^2}}. \tag{2.1}$$

h_e being the Hamiltonian for the 2D confined motion of a free electron perpendicular to the wire:

$$h_e = \frac{P^2_{\rho_e}}{2m_e} + U(\vec{\rho_e}) \tag{2.2}$$

and similarly for h_h. $U(\vec{\rho_e})$ is equal to 0 inside the wire and V outside. Let us introduce the eigenstates of these 2D Hamiltonians

$$h_e|f_{e,p}\rangle = E_{e,p}|f_{e,p}\rangle$$
$$h_h|f_{h,p}\rangle = E_{h,p}|f_{h,p}\rangle,$$

p being a two component index. These eigenstates are explicitly given in Appendix A for cylindrical and rectangular wires. Note that the $|f_{e,p}\rangle$ and $|f_{h,p}\rangle$ wave functions are identical for infinite wire barrier only; otherwise the different electron and hole masses makes them to leak outside the wire differently. In quantum wires with radius R and finite barrier height $V = \hbar^2\nu^2/2mR^2$, the infinite barrier approximation has been shown to be valid when the dimensionless parameter ν is much greater than 1, typically $\nu \geq 5$ [14].

We want to determine the H eigenstates of energy E, namely

$$H|\psi_E\rangle = E|\psi_E\rangle. \tag{2.3}$$

The corresponding wave functions, seen as functions of $\vec{\rho_e}$, can be expanded over the basis of functions made of the $f_{e,p}(\vec{\rho_e})$'s. If we do similarly for $\vec{\rho_h}$, we are led to write:

$$\psi_E(z,\vec{\rho_e},\vec{\rho_h}) = \sum_{p_e,p_h} \varphi_{E,p_e,p_h}(z) f_{e,p_e}(\vec{\rho_e}) f_{h,p_h}(\vec{\rho_h}) \tag{2.4}$$

where the prefactors of this expansion depend on the remaining variables, namely (z,E), and on the indices (p_e,p_h) of the $\vec{\rho_e}$ and $\vec{\rho_h}$ basis. Equation (2.4) formally reads

$$|\psi_E\rangle = \sum_{p_e,p_h} |\varphi_{E,p_e,p_h}\rangle \otimes |f_{e,p_e}\rangle \otimes |f_{h,p_h}\rangle \tag{2.5}$$

where the three kets belong to three different subspaces, z, $\vec{\rho_e}$ and $\vec{\rho_h}$ respectively. By inserting this expression into equation (2.3), we get

$$0 = \sum_{p_e,p_h} \left(E_{e,p_e} + E_{h,p_h} + \frac{P_z^2}{2\mu} - \frac{e^2}{\sqrt{z^2+(\vec{\rho_e}-\vec{\rho_h})^2}} - E \right) |\varphi_{E,p_e,p_h}\rangle \otimes |f_{e,p_e}\rangle \otimes |f_{h,p_h}\rangle. \tag{2.6}$$

2.1 Coupled equations verified by the set of $|\varphi_{E,p_e,p_h}\rangle$'s

If we multiply the above equation by $\langle f_{h,p'_h}| \otimes \langle f_{e,p'_e}|$, we find

$$\left(\frac{P_z^2}{2\mu} - \Delta_{p'_e,p'_h}\right)|\varphi_{E,p'_e,p'_h}\rangle + \sum_{p_e,p_h} V_{p'_e,p'_h;p_e,p_h}|\varphi_{E,p_e,p_h}\rangle = 0 \tag{2.7}$$

where Δ_{p_e,p_h} is the difference between E and the various wire subband energies:

$$\Delta_{p_e,p_h} = E - E_{e,p_e} - E_{h,p_h}. \tag{2.8}$$

V_{p_e,p_h,p'_e,p'_h} is the matrix element of the Coulomb interaction potential between any two of these subband levels:

$$V_{p_e,p_h;p'_e,p'_h} = \left\langle f_{h,p_h}\right| \otimes \left\langle f_{e,p_e}\left| \frac{-e^2}{\sqrt{z^2+(\vec{\rho_e}-\vec{\rho_h})^2}} \right| f_{e,p'_e}\right\rangle \otimes \left| f_{h,p'_h}\right\rangle$$
$$= \int \mathrm{d}\,\vec{\rho_e}\,\mathrm{d}\,\vec{\rho_h}\; f^*_{h,p_h}(\vec{\rho_h}) f^*_{e,p_e}(\vec{\rho_e}) \times \frac{-e^2}{\sqrt{z^2+(\vec{\rho_e}-\vec{\rho_h})^2}} f_{e,p'_e}(\vec{\rho_e}) f_{h,p'_h}(\vec{\rho_h}) \tag{2.9}$$

so that this Coulomb potential is now a function of the variable z only. By extracting the diagonal term from the sum of equation (2.7), we get the set of coupled equations verified by the $|\varphi_{E,p_e,p_h}\rangle$'s as

$$(H_{p_e,p_h} - \Delta_{p_e,p_h})\,|\varphi_{E,p_e,p_h}\rangle + \sum_{(p'_e,p'_h)\neq(p_e,p_h)} V_{p_e,p_h;p'_e,p'_h}|\varphi_{E,p'_e,p'_h}\rangle = 0 \tag{2.10}$$

where H_{p_e,p_h} is a 1D Hamiltonian for the z variable only:

$$H_{p_e,p_h} = \frac{P_z^2}{2\mu} + V_{p_e,p_h;p_e,p_h}. \tag{2.11}$$

2.2 Exact equation verified by one $|\varphi_{E,p_e,p_h}\rangle$ only

Equation (2.10) couples $|\varphi_{E,p_e,p_h}\rangle$ to all the other $|\varphi_{E,p'_e,p'_h}\rangle$'s. If we write a similar equation for each of these other $|\varphi_{E,p'_e,p'_h}\rangle$'s and extract the $|\varphi_{E,p_e,p_h}\rangle$ term from the sum of coupled states, we find that these other $|\varphi_{E,p'_e,p'_h}\rangle$'s can be formally written as

$$|\varphi_{E,p'_e,p'_h}\rangle = \frac{1}{\Delta_{p'_e,p'_h} - H_{p'_e,p'_h}} \times \left(V_{p'_e,p'_h;p_e,p_h}|\varphi_{E,p_e,p_h}\rangle + \sum_{(p''_e,p''_h)\neq(p_e,p_h),(p'_e,p'_h)} V_{p'_e,p'_h;p''_e,p''_h}|\varphi_{E,p''_e,p''_h}\rangle \right). \tag{2.12}$$

If we now insert this $|\varphi_{E,p'_e,p'_h}\rangle$ into the last term of equation (2.10) and we iterate the procedure, we get an equation which contains $|\varphi_{E,p_e,p_h}\rangle$ only. It reads

$$\left(\frac{P_z^2}{2\mu} + \widetilde{V}_{p_e,p_h}\right)|\varphi_{E,p_e,p_h}\rangle = \Delta_{p_e,p_h}|\varphi_{E,p_e,p_h}\rangle \tag{2.13}$$

where $\widetilde{V}$ is the effective "wire potential" for the z motion:

$$\widetilde{V}_{p_e,p_h} = V_{p_e,p_h;p_e,p_h} + \sum_{(p'_e,p'_h)\neq(p_e,p_h)} V_{p_e,p_h;p'_e,p'_h} \frac{1}{\Delta_{p'_e,p'_h} - H_{p'_e,p'_h}} V_{p'_e,p'_h;p_e,p_h} + \sum_{\substack{(p'_e,p'_h)\neq(p_e,p_h) \\ (p''_e,p''_h)\neq(p_e,p_h),(p'_e,p'_h)}} V_{p_e,p_h;p'_e,p'_h} \frac{1}{\Delta_{p'_e,p'_h} - H_{p'_e,p'_h}} V_{p'_e,p'_h;p''_e,p''_h} \times \frac{1}{\Delta_{p''_e,p''_h} - H_{p''_e,p''_h}} V_{p''_e,p''_h;p_e,p_h} + ... \quad (2.14)$$

with Δ_{p_e,p_h}, H_{p_e,p_h} and $V_{p_e,p_h;p'_e,p'_h}$ defined in equations (2.8, 2.11) and (2.9). Note that in the sums, the restrictions on the (p_e,p_h)'s are such that all the V matrix elements are non-diagonal.

Let us stress that this $\widetilde{V}_{p_e,p_h}$ "potential" is somewhat peculiar as it depends on the eigenvalue E through the Δ_{p_e,p_h}'s. It is also non local, as P_z^2 appears in the various H_{p_e,p_h}'s. In spite of these difficulties, equation (2.13) is yet an exact equation. It is however clear that there is no hope to solve the Schrödinger equation (2.13) for quantum wire exciton with this exact $\widetilde{V}_{p_e,p_h}$ potential! We will now see how we can approximate it for narrow wires and estimate the size of the dropped terms.

2.3 Determination of the Coulomb matrix elements $V_{p_e,p_h;p'_e,p'_h}$

Let us first study the Coulomb matrix elements $V_{p_e,p_h;p'_e,p'_h}$ defined in equation (2.9).

a) $z \to \infty$

For z much larger than the wire lateral extension, we immediately find

$$V_{p_e,p_h;p'_e,p'_h}(z\to\infty) \approx -\frac{e^2}{z}\left[\delta_{p_e,p'_e}\delta_{p_h,p'_h} - \frac{a_{p_e,p_h;p'_e,p'_h}}{z^2} + O\left(\frac{1}{z^4}\right)\right] \quad (2.15)$$

as the $|f_n\rangle$'s are orthogonal, the constant $a_{p_e,p_h;p'_e,p'_h}$ being given by

$$a_{p_e,p_h;p'_e,p'_h} = \frac{1}{2}\int \mathrm{d}\,\vec{\rho}_e\,\mathrm{d}\,\vec{\rho}_h \;\; f^*_{e,p_e}(z_e) f^*_{h,p_h}(z_h) \left|\vec{\rho}_e - \vec{\rho}_h\right|^2 \times f_{e,p'_e}(z_e) f_{h,p'_h}(z_h).$$

b) $z \to 0$

When $z \to 0$, the integral of equation (2.9) tends to a finite value. This can be seen by noting that, when $z = 0$, a possible singularity in the integral may come from $\vec{\rho}_e - \vec{\rho}_h = \vec{\rho} \approx \vec{0}$. For such small $\vec{\rho}$'s, $\vec{\rho}_e$ and $\vec{\rho}_h$ can be replaced by $\vec{\rho}' = (\vec{\rho}_e + \vec{\rho}_h)/2$. The integration over the 2D variable $\vec{\rho}$ then shows that $-\frac{e^2}{\rho}$ indeed converges for $\rho \to 0$.

If we now consider the derivative of $V_{p_e,p_h;p'_e,p'_h}(z)$ with respect to z, it writes like equation (2.9), with the ratio replaced by $\frac{e^2 z}{2\left(z^2+(\vec{\rho}_e-\vec{\rho}_h)^2\right)^{3/2}}$. One could naively conclude that $V'_{p_e,p_h;p'_e,p'_h}(z)$ goes to 0 when $z \to 0$ due to the numerator. However here again, a possible singularity may come from $\vec{\rho}_e - \vec{\rho}_h = \vec{\rho} \approx \vec{0}$. The integration over the 2D variable $\vec{\rho}$ of $1/(z^2+\rho^2)^{3/2}$ in fact behaves as $1/z$ for $\rho \to 0$. This compensates the z factor in the numerator so that the derivative of $V_{p_e,p_h;p'_e,p'_h}$ tends to a finite non zero value when $z \to 0$. We thus get

$$V_{p_e,p_h;p'_e,p'_h}(z\to 0) \approx -\frac{e^2}{b_{p_e,p_h;p'_e,p'_h}}\left(1 - \frac{z}{c_{p_e,p_h;p'_e,p'_h}} + O(z^2)\right) \quad (2.16)$$

where $b_{p_e,p_h;p'_e,p'_h}$ and $c_{p_e,p_h;p'_e,p'_h}$ are two finite (non zero) constants of the order of the wire lateral extension R (as R scales the integral (2.9) through all the wavefunctions). The precise value of these constants depends on the shape of the wire through the $h_{e,h}$ eigenstates f_{e,p_e} and f_{h,p_h}. Calculations for some particular wire shapes will be done in Section 3.

c) Diagonal terms

For $(p_e,p_h) = (p'_e,p'_h)$, the integrated quantities are negative for $V_{p_e,p_h;p_e,p_h}(z)$ and positive for $V'_{p_e,p_h;p_e,p_h}(z)$ so that $b_{p_e,p_h;p_e,p_h}$ and $c_{p_e,p_h;p_e,p_h}$ are two positive constants. Similarly, $a_{p_e,p_h;p_e,p_h}$ given in equation (2.15) is also positive. In order to simplify the notations, let us call a_{p_e,p_h}, b_{p_e,p_h} and c_{p_e,p_h} these three constants.

The diagonal matrix elements of the Coulomb potential can thus be written

$$V_{p_e,p_h;p_e,p_h}(z) = -\frac{e^2}{z + b_{p_e,p_h}(z)} \quad (2.17)$$

where $b_{p_e,p_h}(z)$ decreases from b_{p_e,p_h} to 0 when z increases from 0 to ∞.

As shown in Section 3, an amazing fit of these diagonal potentials is obtained by using

$$b_{p_e,p_h}(z) \approx \frac{b_{p_e,p_h}}{\frac{1+\frac{z}{b_{p_e,p_h}}}{1+z\left(\frac{1}{c_{p_e,p_h}}+\frac{b_{p_e,p_h}}{a_{p_e,p_h}}\right)} + z\frac{b_{p_e,p_h}}{a_{p_e,p_h}}}. \quad (2.18)$$

This approximate $b_{p_e,p_h}(z)$, which may look crazy at first, has just been built to reproduce the *two first terms* of the exact V_{p_e,p_h,p_e,p_h}, as given in equations (2.16) and (2.15), for *both* $z \to 0$ and $z \to \infty$; this is why it is indeed so good.

2.4 The most naive quantum wire potential

The most naive quantum wire potential surely corresponds to keep the first term of equation (2.14) only, namely $\widetilde{V}_{p_e,p_h}(z) \approx V_{p_e,p_h;p_e,p_h}(z)$, and in addition to replace $b_{p_e,p_h}(z)$ by a constant $b^*_{p_e,p_h}$.

We can then use Section 1 to get the eigenstates and eigenvalues of the corresponding Schrödinger equation

$$\left(\frac{P_z^2}{2\mu} - \frac{e^2}{|z| + b^*_{p_e,p_h}}\right) |\varphi_{E,p_e,p_h}\rangle = (E - E_{e,p_e} - E_{h,p_h})|\varphi_{E,p_e,p_h}\rangle. \quad (2.19)$$

In the small $b^*_{p_e,p_h}$ limit, we have seen that the eigenvalues of this Schrödinger equation tend to $-R_X/n^2$ with $n = 1, 2, ...$ for excited states, while the energy parameter λ of the ground state goes to zero as $\lambda e^{-1/2\lambda} \approx 2b^*_{p_e,p_h}/a_X$. Consequently exciton excited states (which correspond to wavefunctions with nodes) are found at $E_{e,p_e} + E_{h,p_h} - R_X/n^2$ while ground state excitons are well below $E_{e,p_e} + E_{h,p_h}$.

Such a Schrödinger equation (2.19) a *priori* exists for each quantum wire subband energy $E_{e,p_e} + E_{h,p_h}$. However, except for the lowest wire subband, these eigenstates are not real bound states: as for quantum wells, they are in the exciton continuum of the lowest subband so that they are broadened by Fano effects due to the various $V_{p_e,p_h;p'_e,p'_h}(z)$ couplings, neglected in assuming $\widetilde{V}_{p_e,p_h}(z) \approx V_{p_e,p_h,p_e,p_h}(z)$.

Consequently if we are interested in real bound states, we must consider equation (2.19) for the lowest subband $p_e = p_h = 1$ only, with 1 corresponding to $(n = 1, m = 0)$ for cylindrical wires and $(n_x = n_y = 1)$ for rectangular wires.

Equation (2.19) thus gives the ground state exciton energy at $E_{e1} + E_{h1} - R_X/\lambda_1^2$ with λ_1 solution of $\lambda_1 e^{-1/2\lambda_1} \approx 2b^*_{11}/a_X$. As b^*_{11} is of the order of the wire lateral extension R, the exciton ground state binding energy which writes $\Delta_{11} = -R_X/\lambda_1^2 = -e^{-1/\lambda_1} R_X/(2b^*_{11}/a_X)^2$ scales as $e^{-1/\lambda_1} R_X/(R/a_X)^2$ which is considerably smaller than the intersubband energies which scale as $R_X/(R/a_X)^2$, since λ_1 is very small when R/a_X is small.

2.5 A more elaborate quantum wire potential

A somewhat more elaborate quantum wire potential can be obtained by still keeping the first term of equation (2.14), but by using the exact $V_{11,11}(z)$ as numerically calculated from equation (2.9), or by using the approximate $V_{11,11}(z)$ given in equation (2.17) with $b_{11}(z)$ given in equation (2.18), as it reproduces extremely well the exact $V_{11,11}(z)$. It is clear that for a given wire thickness, there is always one constant b^*_{11} which would give the same energy as the one calculated with $b_{11}(z)$. This can in fact be a way to determine b^*_{11}. However, since the wave function extension is larger for excited states than for the ground state, the best b^*_{11} for the ground state is surely not the best b^*_{11} for excited states: indeed, it optimizes the fit with the exact $V_{11,11}(z)$ for smaller z than the best b^*_{11} for excited states. Consequently, the best b^*_{11} for the ground state has to be closer to $b_{11}(0)$ than the best b^*_{11} for excited states. This will be discussed in more details in Section 3.

2.6 Estimation of the intersubband Coulomb coupling

Let us now come back to the other terms of equation (2.14) dropped by keeping $\widetilde{V}_{11}(z) \approx V_{11,11}(z)$ only. Since all the Coulomb potentials contained in these other terms are non-diagonal, the large z contribution of these dropped terms are in $1/z^6$ at least. So that these intersubband couplings only affect the small z behavior of the effective Coulomb potential, *i.e.* $b_{11}(z \to 0)$.

If we consider the second term in equation (2.14), we may note that, as the second subband corresponds to $p_e = 1$ and $p_h = 2$ (if $m_e < m_h$), we have $\Delta_{12} = \Delta_{11} + E_{h1} - E_{h2} \approx E_{h1} - E_{h2}$ in the small wire thickness limit, since we have shown that the exciton binding energies are much smaller than the wire intersubband energy, even for the ground state. We also see that Δ_{12} is negative as well as all the other $\Delta_{p'_e,p'_h}$'s, their absolute values being larger than Δ_{12}.

In order to estimate the effect of H_{12} appearing in the denominator of the second term of equation (2.14), we can think to expand the functions over which it acts on the eigenstates of H_{12}. As for H_{11}, all the H_{12} bound states energies are small compared to $\Delta_{12} \approx E_{h1} - E_{h2}$ in the narrow wire limit. If we turn to the high energy diffusive states of H_{12}, they may have energies larger than the wire intersubband energy; however as they appear in denominators, the approximation which forgets them tends to overestimate their contribution, which anyway must be small. Consequently, the dominant contribution to the second term of equation (2.14), dropped in keeping $V_{11,11}(z)$ instead of $\widetilde{V}_{11}(z)$, is close to $V_{11,12}(z)^2/(E_{h1} - E_{h2})$. As it is negative, it tends to deepen the wire effective potential, *i.e.* to decrease $b_{11}(z)$. A quantitative calculation of this first correction to $V_{11,11}$ is done in part 3 and an estimate of the wire thickness above which it starts to give a sizeable contribution to the exciton energies will be given.

The third term of equation (2.14) contains 3 non-diagonal potentials and two energy denominators, *i.e.* two intersubband energies. As for the second term of equation (2.14) which modifies the small z behavior of $b_{11}(z)$ by adding a contribution of the order of $V/(E_{h1} - E_{h2})$, this third term adds to the second term of $\widetilde{V}_{11}$ a contribution of the same order. Consequently if we find that the second term of equation (2.14) can indeed be neglected in front of $V_{11,11}$, this will be even more justified for the next order ones. If, on the opposite, we find that it cannot be neglected, we would have to keep *all* the terms in equation (2.14), which is of course totally hopeless.

Consequently, for quantum wires not narrow enough, this procedure based on a Schrödinger equation with a 1D effective Coulomb potential will not be valid anymore. For intermediate thicknesses, we are left with the variational methods only: they can be good for the ground state but most probably, only approximate for excited states [9]. For very large thicknesses, the quantum wire exciton energies must tend to their bulk values. However it will be extremely tricky to get the proper way these asymptotic energies are reached, in view of what we have recently shown for the exciton dead layer in wide quantum wells [15].

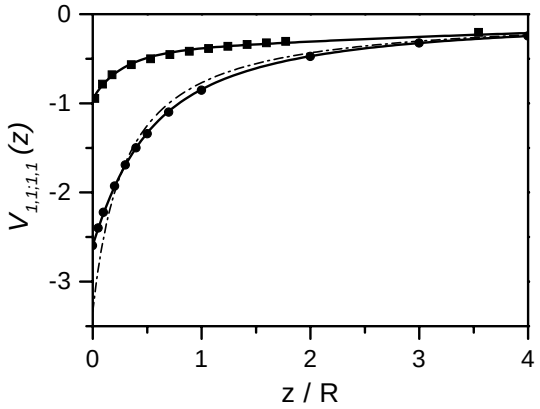

Fig. 5. Effective potential $V_{p_e,p_h,p'_e,p'_h}(z)$ in Rydberg unit $R_X(R/a_X)$ for $p_e = p_h = p'_e = p'_h = 1$ from the numerical calculation of the integral (2.9) (dots) and from its approximate expression equations (2.17, 2.18) (solid line) for cylindrical wire or square wires of same area πR^2: the two results are undistinguishable. The upper curve corresponds to a rectangular wire with a huge anisotropy $\eta = 100$ as numerically calculated (squares) and as obtained from the approximate expressions (2.17, 2.18) (solid line). The fit is amazingly good in all cases. The dashed line corresponds to the potential for a cylindrical wire with a constant broadening $b^* = 0.3R$.

3 Quantitative results

3.1 Approximate effective potential $V_{p_e,p_h;p_e,p_h}(z)$

The effective potential $V_{p_e,p_h;p_e,p_h}(z)$, defined in equation (2.9), averages the Coulomb potential over the confined wavefunctions of the electron and the hole in the subbands (p_e, p_h). We have calculated it numerically for the lowest subbands of cylindrical and rectangular wires. The two lengths of the rectangular wires have been taken as $L_x = R\sqrt{\pi\eta}$ and $L_y = R\sqrt{\pi/\eta}$, so that the cylindrical and rectangular wires have the same area πR^2, the anisotropy of the rectangular wire being controlled by the parameter $\eta = L_x/L_y$. More details on the numerical calculation of this potential $V_{p_e,p_h;p_e,p_h}(z)$ are given in Appendix A.

This effective potential has been approximated by the expression (2.17) with $b(z)$ given by equation (2.18). As shown in Figure 5, the fit is amazing. The three parameters for cylindrical wires of area πR^2 are found to be $a_{1,1} = 0.299\ R$, $b_{1,1} = 0.385\ R$ and $c_{1,1} = 0.599\ R$. It is interesting to note that they are essentially the same as those obtained for a rectangular wire of same area provided that its anisotropy is not too large ($\eta < 1.5$).

In Figure 5, we also show the approximate effective potential for a constant broadening $V(z) = -e^2/(z + b^*)$ with $b^* = 0.3\ R$. We see that this b^* is not quite satisfactory around $z = 0$, *i.e.* where the finite value of the potential is crucial to determine the correct energies.

$V_{p_e,p_h,p'_e,p'_h}(z)$ has also been calculated for the first subbands in order to evaluate the intersubband Coulomb couplings, as shown in the next sections.

3.2 Exciton energies and the best constant broadening parameters b*

As seen in Section 1, the exciton eigenstates are easy to obtain analytically in the frame of a "naively" broadened exciton. The constant broadening parameter b^* has however to be chosen quite precisely in order to obtain correct results. As the approximate potential has to be good over a domain defined by the exciton extension, which depends on the wire radius and the exciton level, the best b^* for a given exciton should *a priori* depend on both. A good way to determine this best b^* is to rewrite the exciton Hamiltonian (2.11) as

$$\left[\frac{P_z^2}{2\mu} - \frac{e^2}{|z| + b^*}\right] + \left[V_{1,1;1,1}(z) + \frac{e^2}{|z| + b^*}\right]. \qquad (3.1)$$

The ground state of the first bracket is known analytically. It corresponds to a wave function $\langle z|\hat{\varphi}_{\lambda,0}\rangle = \Phi_{\lambda,0}(|\zeta| + \beta^*_\lambda)$ with $\zeta = 2z/\lambda a_X$ and $\beta^*_\lambda = 2b^*/\lambda a_X$, the ground state energy parameter being such that $\Phi'_{\lambda,0}(\beta^*_\lambda) = 0$ with $0 < \lambda < 1$, as shown in Section 1. For b^* to be good, the "perturbation" induced by the second bracket of equation (3.1) should give a negligible contribution. At lowest order, this gives

$$D(\lambda) = \left\langle \hat{\varphi}_{\lambda,0} \left| V_{1,1;1,1}(z) + \frac{e^2}{|z| + a_X\ \lambda\ \beta^*_\lambda/2} \right| \hat{\varphi}_{\lambda,0} \right\rangle = 0. \qquad (3.2)$$

Consequently the simplest way to determine the energy parameter of the ground state exciton is to take a λ between 0 and 1, to determine the corresponding β^*_λ by $\Phi'_{\lambda,0}(\beta^*_\lambda) = 0$, to insert these $(\lambda, \beta^*_\lambda)$ into equation (3.2) and to look for λ_0 such that $D(\lambda_0) = 0$. This gives the best b^* for the ground state exciton for this particular wire confinement as $b^*_0 = a_X\ \lambda_0\ \beta^*_{\lambda_0}/2$.

If we now look for excited states with even symmetry, we should do the same, starting with a λ between 1 and 2. $D(\lambda^{(e)}_1) = 0$ then determines the energy parameter $\lambda^{(e)}_1$ of the even first excited states of the exciton, the best broadening for these states being $b^*_{1,e} = a_X\ \lambda^{(e)}_1\ \beta^*_{\lambda^{(e)}_1}/2$.

As for odd first excited states, we should also start with a λ between 1 and 2, get β^*_λ by $\Phi_{\lambda,0}(\beta^*_\lambda) = 0$ and the energy parameter by $D(\lambda^{(o)}_1) = 0$, the best broadening for these states being $b^*_{1,o} = a_X\ \lambda^{(o)}_1\ \beta^*_{\lambda^{(o)}_1}/2$.

Figure 6 shows the best broadening parameter b^*_0 for the exciton ground state in a cylindrical quantum wire of radius R. We see that it is well represented by $b^*_0 \approx 0.33\ R$, in qualitative agreement with [4].

Figure 7 shows the energy parameter λ and the energy E of the ground exciton state and its lowest excited states with even and odd symmetry in the case of cylindrical wires. The square wires of same area give exactly the same result as the potentials $V_{1,1;1,1}(z)$ are identical. In this Figure 7, the excited state exciton energy has been calculated not with $b^*_{1,e}$ or $b^*_{1,o}$, but with the best broadening b^*_0 for ground state excitons, the corresponding λ

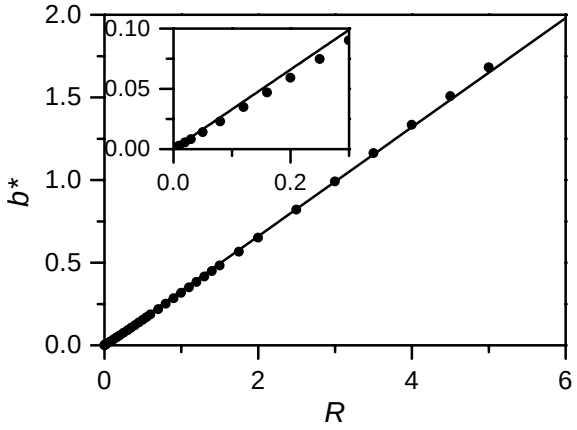

Fig. 6. R dependence of the best broadening parameter b^* for the exciton ground state of a cylindrical wire (circles) in a_X unit. The solid line corresponds to $b^* = 0.33R$. Inset: $b^*(R)$ for R close to 0.

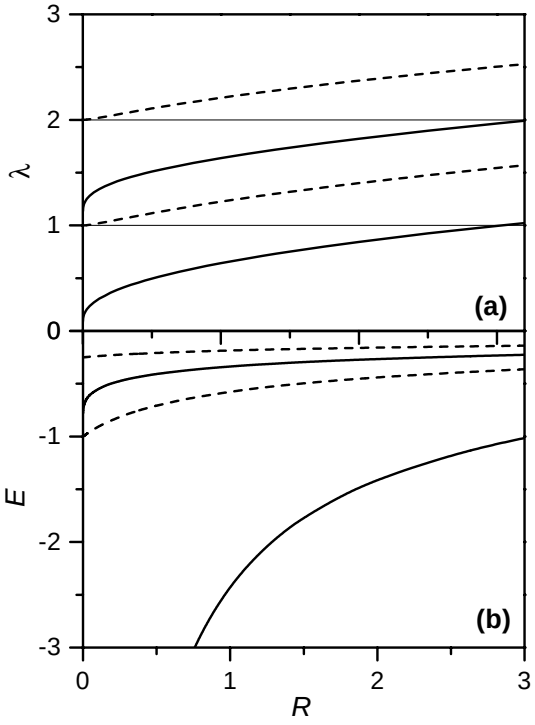

Fig. 7. R dependence of (a) the energy parameter λ and (b) the energy $E = -1/\lambda^2$ in Rydberg units a_X and R_X, for the ground state and the three first excited states of the exciton in the case of cylindrical wires: the solid lines correspond to even states while the dashed lines correspond to odd states. The results for square wires of the same area are identical

parameter being obtained by $\Phi_{\lambda,0}(a_X\ \lambda\ b_0^*/2) = 0$ for odd states and by $\Phi'_{\lambda,0}(a_X\ \lambda\ b_0^*/2) = 0$ for even states.

Figure 8 shows the bare energy of the three lowest exciton excited states $-R_X/\lambda^2$ obtained by using the best ground state broadening b_0^* as well as their corrected values $-R_X/\lambda^2 + D(\lambda)$. We see that the correction $D(\lambda)$ is not negligible (up to 15% over the whole range of R). Figure 8 also shows the same first excited state energies as

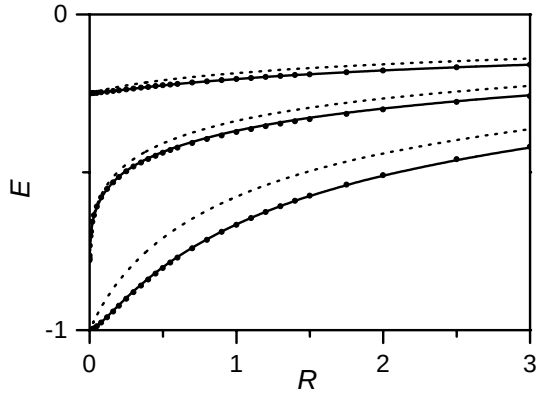

Fig. 8. Comparison of the cylindrical wire exciton energy for the three lowest excited states, obtained with the best broadening b_0^* for ground state excitons (dotted lines), corrected by $D(\lambda)$ (solid lines), and calculated with the broadening b^* such that this correction $D(\lambda)$ is 0 for the exciton state under consideration, *e.g.* $b_{1,e}^*$ or $b_{1,o}^*$ (dots). While $D(\lambda)$ gives a sizeable contribution when compared to the energies calculated with b_0^*, we see that the energies calculated with the best $b_{1,e}^*$ or $b_{1,o}^*$ are essentially the same as the one calculated with b_0^* but corrected by $D(\lambda)$.

calculated with $b_{1,e}^*$ and $b_{1,o}^*$, which are the best broadenings for these even and odd first excited states, as defined by $D(\lambda) = 0$. We see that these energies are essentially the same as the corrected value $-R_X/\lambda^2 + D(\lambda)$ calculated with b_0^*.

3.3 Wire exciton Bohr radius

In order to evaluate the extension of the wavefunction and to study its dependence on the various parameters, we have calculated the "1D exciton Bohr radius", defined by:

$$a_{1D} = \sqrt{\langle \hat{\varphi}_{\lambda,0} \left| z^2 \right| \hat{\varphi}_{\lambda,0} \rangle}. \tag{3.3}$$

The dependence of this Bohr radius on the wire radius R is shown in Figure 9 for cylindrical and square wires. Again, the exciton ground state is singular for small wires, the extension of its wavefunction going to 0. This reflects the strong binding of the exciton ground state. On the opposite, the spatial extensions of the other exciton states remain finite when $R \to 0$. These extensions in fact increase with the level of the excited state, as expected. It can be interesting to note that the scaling of the exciton ground state energy does not vary with the 1D Bohr radius as $E \propto 1/a_{1D}^2$, but rather as $E = 1.25/(a_{1D}/a_X)^{1.66}\ R_X$.

3.4 Effect of the wire anisotropy

The dependence of the exciton energy and Bohr radius on the anisotropy $\eta = L_x/L_y$ of a rectangular wire is shown in Figure 10. The exciton binding energy of the ground state slightly increases when the anisotropy increases, this effect being more pronounced in large area wires. Indeed,

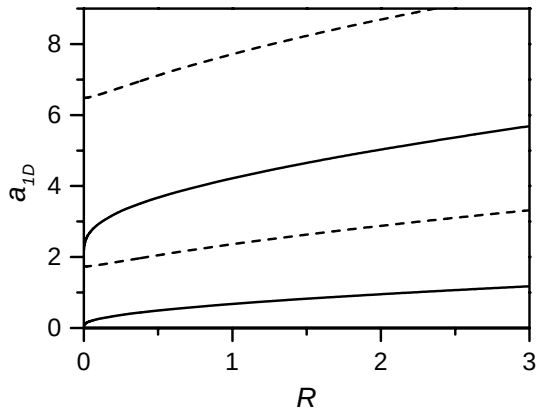

Fig. 9. Bohr radius a_{1D} of the exciton ground state and lowest excited states for cylindrical wires, in a_X unit: even states are shown in solid lines, and odd states in dashed lines. Square wires of the same area give the same results.

the change of the energy in a thin wire ($R = 0.01\ a_X$) when compared to a square wire ($\eta = 1$) is much less dependent on the anisotropy, due to the dramatic divergence of the ground state energy for small radii: the correction induced by the wire anisotropy has a slower divergence for $R \to 0$ than the energy itself. Moreover the energy of the excited states appears to be almost independent of η. This is due to the fact that the wavefunctions of these states are less localized around $z = 0$, where the effective potential strongly depends on the wire shape. This can also be seen from the dependence of the exciton Bohr radius a_{1D} on η, which are presented in Figure 10b: this dependence exactly reflects the energy dependence. Finally, it has to be noted that the decrease of the binding energy for large anisotropies ($\eta > 100$) occurs outside the limits of validity of our model, since the dimension L_x of the corresponding wires becomes much larger than a_X: for rectangular wires, the condition $R < a_X$ is indeed not sufficient to guarantee that the inter-subband coupling is negligible, since both L_x and L_y have to be smaller than a_X.

3.5 Intersubband couplings

In order to evaluate the importance of the intersubband Coulomb couplings, we have calculated the corrections to the energy of the exciton ground state, according to Section 3. As shown in Appendix A, the two main non-diagonal matrix elements for cylindrical wires couple the lowest subband $p = 1$, *i.e.* $(n=1, m=0)$ to the subbands $(n_e=1, m_e=\pm 1; n_h=1, m_h=\mp 1)$, these two states being called $p = 2^{\pm}$, and to $(n_e=1, m_e=0; n_h=2, m_h=0)$, the hole state being called $p = 4$ (see the appendix for these denominations). The dominant change induced by these couplings reads

$$E^{(1)} = \left\langle \hat{\varphi}_{\lambda,0} \left| \frac{V_{1,1,p'_e,p'_h}(z)^2}{E_{p'_e} + E_{p'_h} - E_{e1} - E_{h1}} \right| \hat{\varphi}_{\lambda,0} \right\rangle . \qquad (3.4)$$

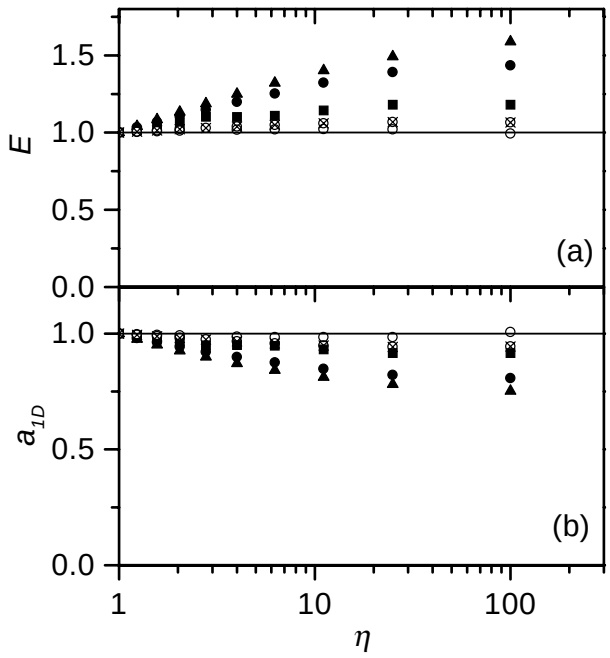

Fig. 10. (a) Anisotropy dependence of the exciton ground state energy for various cylindrical wire radii: $R = 0.01\ a_X$ (plain squares), $R = 0.3\ a_X$ (plain circles), $R = 0.7\ a_X$ (plain triangles). The exciton two first excited states (open and crossed circles) are also represented for $R = 0.3\ a_X$. The unit for the energies has been taken as the value of the exciton ground state energy for $\eta = 1$. (b) Anisotropy dependence of the Bohr radius a_{1D}, the unit being its value for $\eta = 1$. Let us stress that the model proposed in this paper cannot be valid for an anisotropy η as large as 100.

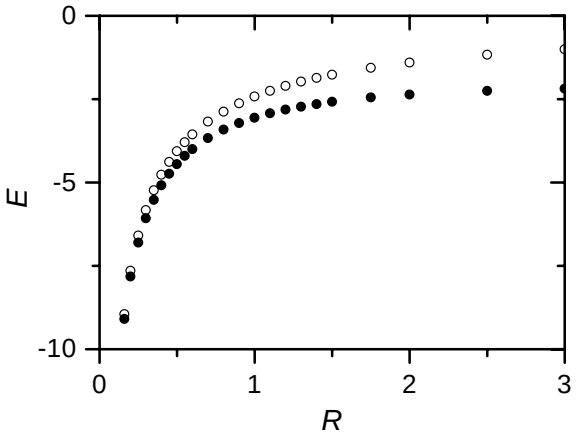

Fig. 11. Ground state exciton energy in R_X unit, with the intersubband couplings correction $E^{(1)}$ as given by equation (3.4) (plain dots) and without it (open dots) for cylindrical wires. R is in a_X unit.

The estimate of the intersubband couplings, shown in Figure 11, has been calculated from these two subbands only. We see that the contribution of this coupling to the exciton energy is not negligible for large wire radii R, as expected. Indeed, the lateral confinement of the electron and the hole in wide wires is not only induced by the single

particle confinement, but also by the Coulomb interaction. In the large R limit, the quantum wire excitons are much like bulk excitons and their energies should not tend to zero as in the single subband model (Fig. 7). The estimate of the inter-subband coupling provides the limit of validity of the present approach, as well as the limit of the one dimensional behavior of the quantum wire. For $R < a_X$ the inter-subband coupling is indeed small compared to the exciton energy so that we can possibly include it as a perturbation. On the opposite, for $R > 2a_X$, the present approach is clearly not valid since the intersubband couplings become of the order of the exciton binding energy itself.

4 Conclusion

In the first part, we have reconsidered the resolution of the hydrogen atom Schrödinger equation in D dimensions, since the one found in textbooks is surprisingly inconsistent, the two supposedly "independent" solutions of this second order differential equation being proportional! Besides the fact that our new resolution is also valid for quantum wires, *i.e.* for D exactly equal to 1 (which was not the case for the previous resolution), it allows to cleanly show that the usual results are (of course) correct: the eigenenergy of the n exciton state in $D = d + 1$ dimensions is indeed equal to $-R_X/(n + d/2)^2$.

In the specific case of quantum wires ($D = 1$, *i.e.* $d = 0$), the exciton ground state $n = 0$ in this approach has an infinite negative energy, the Schrödinger equation for $D = 1$ being highly singular: only odd states are found for the exact 1D exciton relative motion.

A physically more interesting approach to the quantum wire excitons is to take into account the finite size of the wire through the confinement of the electrons and holes. The effective Coulomb potential felt by the exciton relative motion along the wire depends on the wavefunctions of the carriers in the confined directions. The two main characteristics of this confinement — the area and the anisotropy of the cross-section of the wire — have been introduced in the particular cases of cylindrical and rectangular wires, and the dependence of the exciton binding energy on these parameters has been calculated.

This effective Coulomb potential for the relative motion along the wire has however to be determined very carefully in order to possibly obtain meaningfull values for the ground state exciton energy. For that, we found a way to write the exact "potential" felt by the relative motion. This allowed us to securely extract its leading term for narrow wires and to estimate the effects of the dropped terms on the exciton energies.

Through a well defined procedure for the obtention of the "best" constant broadening for this effective Coulomb potential, we succeeded to write the exciton eigenstates in an analytic way, so that these wave functions can easily be handled.

We also evaluated the exciton Bohr radius, which contains most of the physical properties of the exciton ground state. Finally we investigated the limits of the simple single subband approach and we showed that it is valid for wire radius smaller than the 3D Bohr radius. For larger wires, the intersubband couplings have to be included in a non-perturbative way.

Appendix A

Two simple quantum wire geometries have been studied quantitatively in this work, namely cylindrical and rectangular wires. In both cases, the wave functions for the confinement of electrons and holes perpendicular to the wire direction are known analytically, even for finite barriers [14]. The infinite barrier approximation has been shown [14] to be valid when the dimensionless parameter ν characterizing the barrier height $V = \hbar^2\nu^2/2mR^2$ is much larger than 1, typically $\nu \geq 5$. In the following, we will however consider infinite barriers for simplicity, since the electron and hole wavefunctions are then identical. By considering rectangular quantum wires of sizes $L_x = R\sqrt{\pi\ \eta}$ and $L_y = R\sqrt{\pi/\eta}$, we can easily obtain its dependence on the anisotropy $\eta = L_x/L_y$.

A.1 Wave functions

a) Cylindrical wires of radius R

The subbands are characterized by two quantum numbers $n = (1, 2, 3...)$ and $\pm m$, with $m = (0, 1, 2...)$. The wavefunctions of the h_e and h_h eigenstates are given in terms of Bessel functions J_m by

$$f_{e,(n,\pm m)}(\rho,\theta) = f_{h,(n,\pm m)}(\rho,\theta) = \frac{J_m(z_m^{(n)}\rho/R)}{\sqrt{\pi}\ R\ J_{m+1}(z_m^{(n)})}\ \mathrm{e}^{\pm \mathrm{i}m\theta}\ \Theta(R-\rho)$$

where Θ is the Heavyside function and $z_m^{(n)}$ is the n^{th} zero of the Bessel function J_m. Their eigenenergies are $E_{e,(n,\pm m)} = z_m^{(n)}\hbar^2/2m_eR^2$ for electrons, with the electron mass m_e replaced by m_h for holes. For simplicity, the lowest subbands have been denoted by a single index p and classified according to their increasing energies: this leads to call $p = 1$ the state $(n = 1, m = 0)$, which corresponds to $z_0^{(1)} \approx 2.40$. In a similar way, we have called $p = 2^{\pm}$ the two states $(n = 1, m = \pm 1)$ corresponding to $z_1^{(1)} \approx 3.83$, $p = 3^{\pm}$ the two states $(n = 1, m = \pm 2)$ corresponding to $z_2^{(1)} \approx 5.14$, $p = 4$ the state $(n = 2, m = 0)$ corresponding to $z_0^{(2)} \approx 5.52$ and so on...

b) Rectangular wires (L_x, L_y)

The confinements in the two lateral directions commute for infinite barriers. The subbands are characterized by two quantum numbers $n_x = (1, 2, 3...)$

and $n_y = (1, 2, 3...)$. The wavefunctions of the electron and hole eigenstates are given by

$$f_{e,(n_x,n_y)}(x,y) = f_{h,(n_x,n_y)}(x,y) = g_{n_x,L_x}(x) g_{n_y,L_y}(y),$$

with

$$g_{n,L}(u) = \begin{cases} \sqrt{\dfrac{2}{L}} \cos\left(n\dfrac{\pi u}{L}\right) \Theta(L-|u|) & \text{for odd } n \\ \sqrt{\dfrac{2}{L}} \sin\left(n\dfrac{\pi u}{L}\right) \Theta(L-|u|) & \text{for even } n. \end{cases}$$

Their energies are $E_{e,(n_x,n_y)} = (\hbar^2/2m_e)\ (n_x^2/L_x^2 + n_y^2/L_y^2)$ for electrons, with m_e replaced by m_h for holes. The lowest rectangular wire subband corresponds to $n_x = n_y = 1$, which will be called $p = 1$; the next one corresponds to $n_x = 2, n_y = 1$ if $L_x > L_y$, *i.e.* $\eta > 1$, we will call it $p = 2$ and so on...

A.2 Matrix elements of the Coulomb interaction

a) For cylindrical wires,
the numerical calculation of the diagonal matrix elements ($p'_e = p_e = (n_e, m_e), p'_h = p_h = (n_h, m_h)$) of the Coulomb interaction given by equation (2.9) ends by a double numerical integration: we do find

$$V_{p_e,p_h;p_e,p_h}(z) = \iint_0^R \rho_e \mathrm{d}\rho_e \rho_h \mathrm{d}\rho_h \frac{J^2_{m_e}(z^{(n_e)}_{m_e}\rho_e/R)\ J^2_{m_h}(z^{(n_h)}_{m_h}\rho_h/R)}{\pi^2 R^4 J^2_{m_e+1}(z^{(n_e)}_{m_e}) J^2_{m_h+1}(z^{(n_h)}_{m_h})}$$
$$\times 2\pi \int_0^{2\pi} \mathrm{d}\theta \frac{-e^2}{\sqrt{z^2+\rho_e^2+\rho_h^2-2\rho_e\rho_h\cos(\theta)}}$$
$$= \frac{8}{\pi J^2_{m_e+1}(z^{(n_e)}_{m_e}) J^2_{m_h+1}(z^{(n_h)}_{m_h})} \frac{-e^2}{R}$$
$$\times \iint_0^1 u_e \mathrm{d}u_e u_h \mathrm{d}u_h \frac{J^2_{m_e}(z^{(n_e)}_{m_e}u_e)\ J^2_{m_h}(z^{(n_h)}_{m_h}u_h)}{\sqrt{(z/R)^2+(u_e+u_h)^2}}$$
$$\times K\left(\frac{4u_eu_h}{(z/R)^2+(u_e+u_h)^2}\right),$$

where K is the complete elliptic integral of the first kind.

The non-diagonal matrix elements of the Coulomb interaction differ from 0 for $m_e + m_h = m'_e + m'_h$ only, due to the $\mathrm{e}^{\mathrm{i}m\theta}$ dependence of their wave function. The lowest subband for electrons and holes, $p = 1$ which corresponds to $(n = 1, m = 0)$ is therefore coupled to the electron-hole subbands $(n'_e, m'_e), (n'_h, m'_h = -m'_e)$. The two main corrections to the single subband potential $V_{1,1;1,1}(z)$ in equation (2.14) are thus associated to the coupling with the subbands $(p'_e = 2^+, p'_h = 2^-)$ and $(p'_e = 1, p'_h = 4)$. Their energy differences with the lowest subbands are respectively $(z^{(1)}_1 - z^{(1)}_0)(1/m_e + 1/m_h)\hbar^2/2R^2$ and $(z^{(2)}_0 - z^{(1)}_0)\hbar^2/2m_hR^2$, if we assume $m_e < m_h$. The two corresponding coupling are given by:

$$V_{(1,1;p'_e=2^+,p'_h=2^-)}(z) = \iint_0^R \rho_e \mathrm{d}\rho_e\ \rho_h \mathrm{d}\rho_h$$
$$\times \frac{2J_0^2(z^{(1)}_0\rho_e/R)\ J_0(z^{(1)}_0\rho_h/R)\ J_0(z^{(2)}_0\rho_h/R)}{\pi\ R^4\ J_1^3(z^{(1)}_0)\ J_1(z^{(2)}_0)}$$
$$\times \frac{-4e^2}{\sqrt{z^2+(\rho_e+\rho_h)^2}}\ K\left(\frac{4\rho_e\rho_h}{z^2+(\rho_e+\rho_h)^2}\right)$$

$$V_{(1,1;p'_e=1,p'_h=4)}(z) = \iint_0^R \rho_e \mathrm{d}\rho_e\ \rho_h \mathrm{d}\rho_h$$
$$\times \frac{2\ J_0(z^{(1)}_0\rho_e/R)\ J_0(z^{(1)}_0\rho_h/R)}{\pi\ R^4\ J_1^2(z^{(1)}_0)}$$
$$\times \frac{J_1(z^{(1)}_1\rho_e/R)\ J_1(z^{(1)}_1\rho_h/R)}{J_2^2(z^{(1)}_1)}$$
$$\times \int_0^{2\pi} \mathrm{d}\theta \mathrm{e}^{\mathrm{i}\theta} \frac{-e^2}{\sqrt{z^2+\rho_e^2+\rho_h^2-2\rho_e\rho_h\cos(\theta)}},$$

where $\theta = \theta_e - \theta_h$. The integral over θ in the last equation can be expressed analytically as a function of the complete elliptic integral E and the complete elliptic integral of the first kind K.

b) For rectangular wires,
the calculation of the matrix elements of the Coulomb interaction involves a quadruple integration over the coordinates (x_e, y_e, x_h, y_h). The diagonal elements $p_e = p'_e = (n_{e,x}, n_{e,y}), p_h = p'_h = (n_{h,x}, n_{h,y})$ can be written as:

$$V_{p_e,p_h}(z) = \int_{-L_y/2}^{L_y/2} \mathrm{d}y_e \int_{-L_y/2}^{L_y/2} \mathrm{d}y_h g_{n_{e,y},L_y}(y_e)^2 g_{n_{h,y},L_y}(y_h)^2$$
$$\times \frac{w_{n_{e,x},n_{h,x}}(\sqrt{z^2+(y_e-y_h)^2}/L_x)}{L_x}$$

$$w_{n_{e,x},n_{h,x}}(v) = \int_{-1/2}^{1/2} \mathrm{d}u_e \int_{-1/2}^{1/2} \mathrm{d}u_h \frac{-e^2 g_{n_{e,x},1}(u_e)^2 g_{n_{h,x},1}(u_h)^2}{\sqrt{v^2+(u_e-v_h)^2}}.$$

The non-diagonal elements, which can be written in the same way, do not follow any selection rule. Assuming $m_e < m_h$ and $L_x < L_y$, the dominant inter-subband contribution of the lowest subband $(n_{e,x} = n_{h,x} = n_{e,y} = n_{h,y} = 1)$ comes from $(n_{e,x} = n_{h,x} = n_{e,y} = 1, n_{h,y} = 2)$, the energy separation between these subbands being $3\hbar^2/2m_hR^2$.

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