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# Variational approach to soft-Coulomb potential in low-dimensional quantum systems

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## Abstract

The variational method is used to obtain the ground- and first-excited states for soft-Coulomb central potential,  $1/\sqrt{r^2 + d^2}$ , characterized by a bias distance  $d$ , taken into account as a fixed parameter. Applications are presented for spatially indirect excitons, i.e. photo-generated electron-hole ( $e-h$ ) bound pairs, where the two charges are kept separated in two different regions of a heterostructure. We consider one- or two-dimensional systems, namely quantum wires or wells, respectively, and compare the results with numerical calculations obtained by finite-difference diagonalization of the Hamiltonian. An explicit example is given for GaAs-based heterostructures.

## I. INTRODUCTION

Finding the eigenstates of an hydrogen atom is a fundamental application in elementary quantum mechanics. The hydrogenic problem has also important applications in semiconductor physics.<sup>1</sup> Indeed, the same Schrödinger equation with a bare Coulomb potential  $\sim 1/r$ , but with a crystal renormalized mass and electric charge, is used to estimate 1) the electronic states of a shallow impurity and 2) the excitonic states, i.e. the bound state formed by an electron, excited to the conduction band through the gap, and its hole left in the valence band.<sup>2</sup> It is relevant that exact analytical solutions of the hydrogenic problem exist also in 2D and 1D.<sup>3</sup> This is not only an academic exercise in quantum mechanics, but also a problem of great interest, since in semiconductor heterostructures, such as quantum wells and quantum wires, the dynamics of the carriers can be effectively frozen by quantum confinement in one or more directions.

Unlike the hydrogenic problem with the bare Coulomb interaction, exact solutions of the Schrödinger equation do not exist for the *soft-Coulomb potential*  $V(r) \sim 1/\sqrt{r^2 + d^2}$ , obtained from the bare Coulomb potential  $1/r$  by including the parameter  $d$  as a fixed bias distance. This potential is commonly used in semiconductor physics since 1) it overcomes divergence issues, which arise, in one-dimensional systems, in the bare Coulomb potential at the origin,  $r = 0$ , and where  $d$  in this case is taken as a fixed cut-off parameter being of the order of the confinement lateral extension, and 2) it represents the coupling of an electron confined in a layer to a hole (or to a ionized impurity) sitting in a different layer, a distance  $d$  apart (see Fig. 1). Such an excitonic state is called spatially indirect exciton (SIX). The physics of SIXs has been widely investigated due to their intrinsic bosonic character for the observation of macroscopic quantum condensates,<sup>4,5</sup> as well for new classes of opto-electronic devices: the intrinsic coupling of  $e$ - $h$  pairs to photons, and the extended lifetime and permanent dipole of SIXs – due to the non vanishing separation  $d$  between the two charges – allows for long-path exciton transport (see, e.g., Ref. 6).

Of course, the solution of the Schrödinger problem with the soft Coulomb potential in 1D or 2D can be found numerically with limited effort, e.g., by direct discretization of space on a grid, but of course it lacks the greater physical intuition given by a closed-form analytical solution.<sup>7</sup>

In this paper we propose a variational approach of the Schrödinger problem with soft

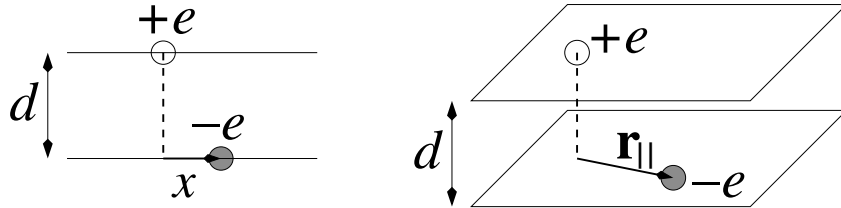


FIG. 1. Sketch of the hydrogen-like model for low-dimensional systems, if the two particles sit in different layers, separated by a vertical distance  $d$ . 1D (left) and 2D (right) configurations.

Coulomb potential. The variational approach is typically taught in undergraduate courses due to both its simplicity and its capacity to provide approximate but transparent solutions to quantum equations, including complex many-body problems, exploiting one's physical intuition of the problem. Furthermore, from the semiconductor physicist's standpoint, the variational approach has been successfully adopted to study excitonic effects and more complex excitation (biexcitons, trions) in low dimensional systems, like, e.g., carbon nanotubes or quantum dots.<sup>8-11</sup> Therefore, we expected it to be suitable for the study of SIXs in semiconductor heterostructures as well.

In this paper we exploit the soft character at short range of the interaction potential using simple harmonic oscillator eigenstates as *ansätze*; this leads to a simple analytical treatment but with very accurate results. We do so both in 1D and 2D and for the ground and first excited states. The variational approach is typically used for the ground state, but it can also be used for excited states if a set of mutually orthogonal and normalizable trial functions is exploited.<sup>12</sup> Excited states are required if optical matrix elements or response functions need to be calculated in an approximate fashion.

We provide the implicit equations for the variational parameters which can be autonomously used by undergraduate students with a mathematical software or easily programmed.<sup>13</sup> We also provide their numerical solution and analyze the accuracy of the variational solutions down to the  $d \rightarrow 0$  limit. As an application to semiconductor physics, we provide the binding energies of SIXs in GaAs-based coupled quantum wires and wells.

In Sec. II, after a short summary on the variational method, we exploit it to find the equations whose solutions are the optimal variational parameters; these are then used to obtain the variational eigenenergies and the related eigenfunctions, for 1D and 2D systems.

Section III is subdivided in two subsections: in Sec. III A we report the results of the variational method in dimensionless units, with the energies expressed in effective Rydbergs and the lengths in Bohr radii, while in Sec. III B we give explicit values concerning GaAs-based systems. A comparison is performed between the eigenenergies/states obtained within the variational and the numerically exact diagonalization of the Hamiltonian. Finally, in Sec. IV, we draw the main conclusions about the present work.

## II. METHOD

The variational method is usually exploited to find the ground state of a quantum Hamiltonian. The method still holds to find excited eigenstates if a proper choice of mutually orthogonal, normalized, trial functions is provided.<sup>12</sup>

The variational method is here adopted within its undergraduate-course formulation:

1. Choose a trial function (*ansatz*)  $\phi_i(\mathbf{r}; \beta_i)$ , dependent on the variational parameter  $\beta_i$  and on the coordinates  $\mathbf{r}$ , for the  $i$ -th state.
2. Calculate the expectation value

$$\begin{aligned} \varepsilon_i(\beta_i) &\equiv \langle \phi_i(\beta_i) | H | \phi_i(\beta_i) \rangle \\ &= \int \phi_i^*(\mathbf{r}; \beta_i) H \phi_i(\mathbf{r}; \beta_i) d\mathbf{r} \end{aligned} \quad (1)$$

of the Hamiltonian  $H$  on the state  $\phi_i$

3. Solve the equation

$$\frac{\partial \varepsilon_i}{\partial \beta_i} = 0 \quad (2)$$

to find the specific (*optimal*) value  $\beta_i$  for which  $\varepsilon_i$  has an extremum.

In what follows, we apply – for one- and two-dimensional systems – the variational method to a Hamiltonian ( $m$  is the reduced effective mass of the system)

$$H = -\frac{\hbar^2 \nabla^2}{2m} + V(r) \quad (3)$$

characterized by the soft Coulomb potential

$$V(r) = -k \frac{1}{\sqrt{r^2 + d^2}} \quad (4)$$

where  $d$  is the bias separation (or softening parameter), and  $k$  is the Coulomb constant. Here we take  $k \equiv e^2/(4\pi\epsilon_0\epsilon_r)$  where  $\epsilon_0$  is the dielectric permittivity in vacuo, and  $\epsilon_r$  the relative dielectric permittivity of the material.

### A. One-dimensional systems

In 1D, the Hamiltonian in Eq. (3) is

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x), \quad (5)$$

where

$$V(x) = -k \frac{1}{\sqrt{x^2 + d^2}}. \quad (6)$$

By taking the ground state of the 1D quantum harmonic oscillator,

$$\phi_0(x) = \left(\frac{\beta_0}{\pi}\right)^{1/4} e^{-\beta_0 x^2/2}, \quad (7)$$

as the normalized *ansatz* ground state, we have

$$\varepsilon_0 = \frac{\hbar^2}{4m} \beta_0 - k \sqrt{\frac{\beta_0}{\pi}} e^{d^2 \beta_0/2} K_0 \left(\frac{d^2 \beta_0}{2}\right) \quad (8)$$

where  $\beta_0$  is the variational parameter, and  $K_0$  is the modified Bessel function of second kind of order 0.

The derivative of  $\varepsilon_0$  with respect to the variational parameter is

$$\frac{\partial \varepsilon_0}{\partial \beta_0} = \frac{\hbar^2}{4m} - \frac{k}{2\sqrt{\beta_0\pi}} \exp\left(\frac{d^2 \beta_0}{2}\right) \left[ (1 + d^2 \beta_0) K_0 \left(\frac{d^2 \beta_0}{2}\right) - d^2 \beta_0 K_1 \left(\frac{d^2 \beta_0}{2}\right) \right], \quad (9)$$

$K_0$  and  $K_1$  being modified Bessel functions of second kind of order 0 and 1, respectively.

We exploit the variational method to minimize  $\varepsilon_0$ : The optimal parameter is obtained from the solution of the transcendent equation  $\partial \varepsilon_0 / \partial \beta_0 = 0$ , which can be re-written more compactly as

$$\frac{e^{t_0/2}}{\sqrt{t_0}} \left[ (1 + t_0) K_0 \left(\frac{t_0}{2}\right) - t_0 K_1 \left(\frac{t_0}{2}\right) \right] = \frac{\sqrt{\pi}}{2} \frac{a_B}{d} \quad (10)$$

where  $a_B \equiv 4\pi\epsilon_0\epsilon_r \hbar^2 / (e^2 m) = \hbar^2 / (mk)$  is the effective Bohr radius, and  $t_0 \equiv d^2 \beta_0$  is a dimensionless quantity.

Analogously, the first excited state can be computed through the variational principle, with the *ansatz*

$$\phi_1(x) = \left(\frac{\beta_1}{\pi}\right)^{1/4} (\sqrt{2\beta_1} x) e^{-\beta_1 x^2/2}, \quad (11)$$

giving

$$\varepsilon_1 = \frac{3\hbar^2}{4m}\beta_1 - k\sqrt{\beta_1}U\left(\frac{1}{2}, 0, d^2\beta_1\right), \quad (12)$$

where  $U$  is the Tricomi confluent hypergeometric function.<sup>14</sup> Hence, we have

$$\frac{\partial\varepsilon_1}{\partial\beta_1} = \frac{3\hbar^2}{4m} + \frac{k}{2\sqrt{\pi\beta_1}}d^2\beta_1e^{d^2\beta_1/2} \left[ (2d^2\beta_1 + 3)K_0\left(\frac{d^2\beta_1}{2}\right) - (2d^2\beta_1 + 1)K_1\left(\frac{d^2\beta_1}{2}\right) \right], \quad (13)$$

leading to the following equation for the optimal  $\beta_1$ .<sup>15</sup>

$$\frac{1}{\sqrt{t_1}} \left[ U\left(\frac{1}{2}, 0, t_1\right) - t_1U\left(\frac{3}{2}, 1, t_1\right) \right] = \frac{3}{2} \frac{a_B}{d} \quad (14)$$

where  $t_1 \equiv d^2\beta_1$ .

The solution to Eqs. (10) and (14) are the optimal variational parameters  $\beta_0$  and  $\beta_1$  as functions of the bias distance  $d$  and the material parameters  $m$  and  $\epsilon_r$ . They can be obtained – numerically – with the aid of standard computational tools, like Wolfram Alpha or Mathematica.<sup>13,16</sup>

The substitution of the optimal values for  $\beta_0$  and  $\beta_1$  in Eqs. (8) and (12) gives the variational ground- and first-excited-state energies,  $\varepsilon_0$  and  $\varepsilon_1$ , respectively.<sup>17</sup>

## B. Two-dimensional systems

For the 2D case, the pair interaction is

$$V(x, y) = -k \frac{1}{\sqrt{x^2 + y^2 + d^2}} \quad (15)$$

The *ansatz* ground state is

$$\phi_0(x, y) = \left(\frac{\beta_0}{\pi}\right)^{1/2} e^{-\beta_0(x^2+y^2)/2}, \quad (16)$$

from which

$$\varepsilon_0 = \frac{\hbar^2\beta_0}{2m} - k\sqrt{\pi\beta_0}e^{d^2\beta_0} \operatorname{erfc}\left(d\sqrt{\beta_0}\right), \quad (17)$$

where  $\operatorname{erfc} = 1 - \operatorname{erf}$  is the complementary error function. We thus have

$$\frac{\partial\varepsilon_0}{\partial\beta_0} = \frac{\hbar^2}{2m} + kd \left[ 1 - \frac{\sqrt{\pi}(1 + 2d^2\beta_0)e^{d^2\beta_0} \operatorname{erfc}(d\sqrt{\beta_0})}{2d\sqrt{\beta_0}} \right], \quad (18)$$

after which the extremal condition is given by

$$\frac{\sqrt{\pi} (1 + 2t_0) e^{t_0} \operatorname{erfc}(\sqrt{t_0})}{2\sqrt{t_0}} = \frac{1}{2} \frac{a_B}{d} + 1. \quad (19)$$

The first excited eigenstates can be represented by the following *ansätze*

$$\phi_{1x}(x, y) = \left(\frac{\beta_1}{\pi}\right)^{1/2} (\sqrt{2\beta_1}x) e^{-\beta_1(x^2+y^2)/2} \quad (20)$$

and

$$\phi_{1y}(x, y) = \left(\frac{\beta_1}{\pi}\right)^{1/2} (\sqrt{2\beta_1}y) e^{-\beta_1(x^2+y^2)/2} \quad (21)$$

which are, by symmetry, degenerate, and mutually orthogonal.

The expectation value of the energy on one of these states is

$$\varepsilon_1 = \frac{\hbar^2 \beta_1}{m} - \frac{k}{2} \sqrt{\pi \beta_1} \left[ 2 \frac{d\sqrt{\beta_1}}{\sqrt{\pi}} + (1 - 2d^2 \beta_1) e^{d^2 \beta_1} \operatorname{erfc}(d\sqrt{\beta_1}) \right], \quad (22)$$

and its derivative with respect to the variational parameter  $\beta_1$  is

$$\frac{\partial \varepsilon_1}{\partial \beta_1} = \frac{\hbar^2}{m} - k \left\{ \frac{d}{2} (1 + 2d^2 \beta_1) + e^{d^2 \beta_1} \operatorname{erfc}(d\sqrt{\beta_1}) \sqrt{\frac{\pi}{16\beta_1}} [1 - 4d^2 \beta_1 (1 + d^2 \beta_1)] \right\}. \quad (23)$$

Therefore, the extremal condition reads

$$(1 + 2t_1) + e^{t_1} \operatorname{erfc}(\sqrt{t_1}) \frac{\sqrt{\pi}}{2\sqrt{t_1}} [1 - 4t_1 (1 + t_1)] = \frac{2a_B}{d} \quad (24)$$

One could in principle go on with higher levels than the first excited state, taking as *ansätze* the higher eigenfunctions of the quantum harmonic oscillator Hamiltonian. The variational principle still holds, since such states are mutually orthogonal. The explicit derivation is straightforward, and not reported here.

### III. RESULTS

#### A. Dimensionless analysis

By adopting the effective Bohr radius,  $a_B$ , and the effective Rydberg,  $\operatorname{Ry} \equiv me^4/(32\pi^2 \epsilon_0^2 \epsilon_r^2 \hbar^2) = k/(2a_B)$ , as units for length and energy, respectively, we can obtain material-independent expressions for the optimal variational parameters and eigenenergies.



In what follows we shall use capital letters  $D \equiv d/a_B$  and  $L_i \equiv l_i/a_B = 1/(a_B\sqrt{\beta_i})$ , to denote the dimensionless bias separation and the width of the variational states, respectively, *in units of  $a_B$* .

It is straightforward to show that the 1D variational eigenenergies Eqs. (8), (12) can be recast as

$$\varepsilon_0 = \frac{\text{Ry}}{L_0} \left\{ \frac{1}{2L_0} - \frac{2}{\sqrt{\pi}} e^{(D/L_0)^2/2} K_0 \left( \frac{(D/L_0)^2}{2} \right) \right\}, \quad (25)$$

and

$$\varepsilon_1 = \frac{\text{Ry}}{L_1} \left\{ \frac{3}{2L_1} - 2U \left( \frac{1}{2}, 0, (D/L_1)^2 \right) \right\}, \quad (26)$$

respectively.

Analogously, for the 2D case we have that Eqs. (17) and (22) are recast into

$$\varepsilon_0 = \frac{\text{Ry}}{L_0} \left\{ \frac{1}{L_0} - 2\sqrt{\pi} e^{(D/L_0)^2} \text{erfc}(D/L_0) \right\}, \quad (27)$$

and

$$\varepsilon_1 = \frac{\text{Ry}}{L_1} \left\{ \frac{2}{L_1} - \left[ 2\frac{D}{L_1} + \sqrt{\pi} (1 - 2(D/L_1)^2) e^{(D/L_1)^2} \text{erfc}(D/L_1) \right] \right\}. \quad (28)$$

The optimal values for  $L_i = L_i(D)$ , solution of the variational problem, are given in Fig. 2(top). Fig. 2(bottom), we show instead the eigenenergies  $\varepsilon_i$  obtained within the variational method (solid lines), and numerically (dashed lines). The latter are obtained via numerical diagonalization of the Hamiltonian, written in second-order-accurate, finite-difference shape. For the numerical calculations, we used ARPACK libraries,<sup>18</sup> and a spatial grid of density  $\approx 7$  point/ $a_B$  for each axis. We see that the variational method gives results for  $\varepsilon_i$  which depart from the exact ones only for  $D \ll 1$ . Moreover, for  $D = 0$ , where  $V(r)$  reduces to the true-Coulomb potential, exact solutions exist both in 1D<sup>19</sup> and in 2D<sup>20</sup>:

$$\begin{cases} (1\text{D}) \rightarrow \varepsilon_i = -\text{Ry}/i^2 \\ (2\text{D}) \rightarrow \varepsilon_i = -\text{Ry}/(i + 1/2)^2 \end{cases} \quad (29)$$

with  $i = 0, 1, 2, \dots$

Note that the ground-state energy for 1D systems diverges for vanishing  $D$ , while, in 2D, it is  $-4\text{Ry}$ . The red thin (thick) arrow in Fig. (2) indicates the  $D = 0$  energy for the first excited state for 1D (2D) system,  $\varepsilon_1(D = 0) = -1\text{Ry}$  ( $-4/9\text{Ry}$ ). While numerical calculations are able to reproduce the correct results at  $D = 0$ , the variational method overestimate it by  $\approx 20\%$ .

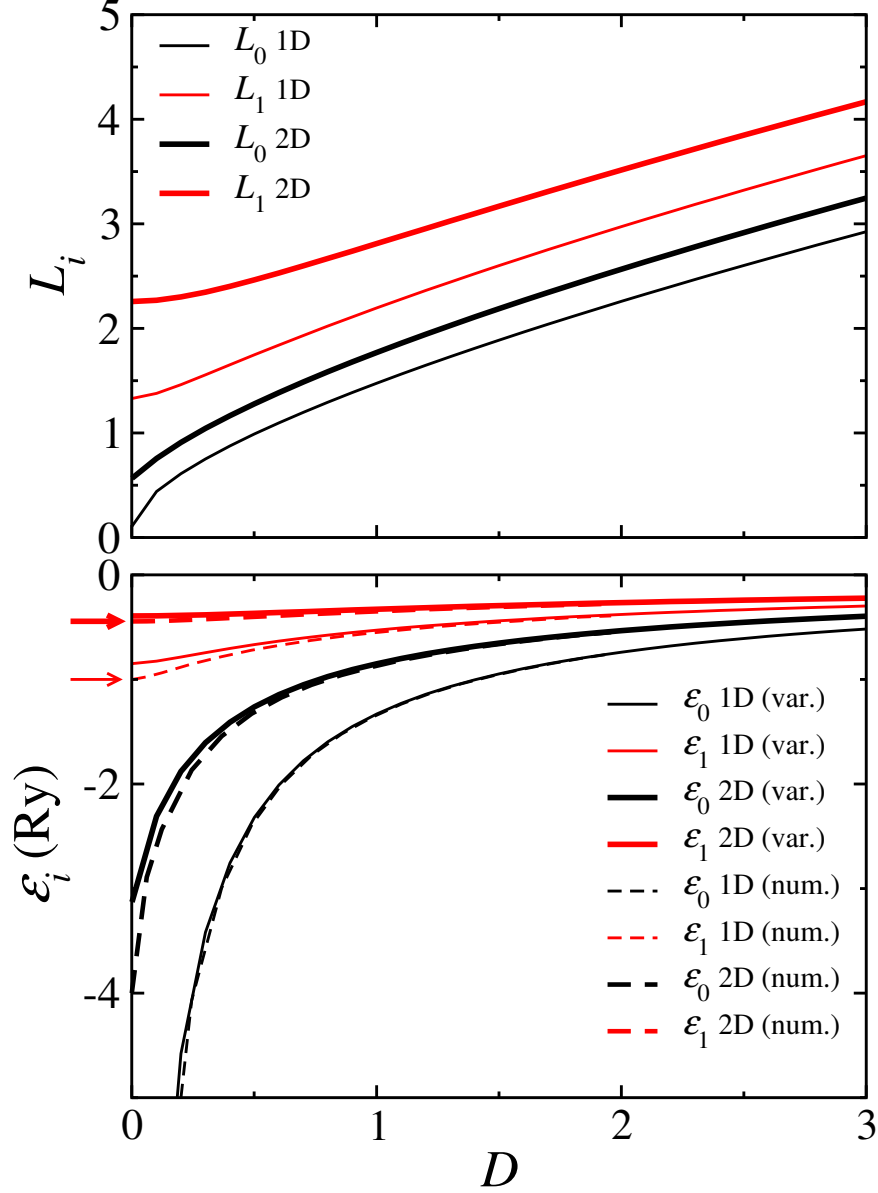


FIG. 2. Top panel: behavior of 1D (thin lines) and 2D (thick lines) variational spatial extension for the ground state,  $L_0$  (black), and the first excited state,  $L_1$  (red), as a function of the bias distance  $D$ . Bottom panel: behavior of variational (solid), and numerical (dashed) energy levels  $\varepsilon_0$  (black) and  $\varepsilon_1$  (red) as a function of  $D$ , in 1D (thin) and 2D (thick). The thin (thick) red arrow points at the  $D = 0$  energy limit for the first excited state for 1D (2D) system, i.e.  $\varepsilon_1 = -1$  Ry ( $-4/9$  Ry).

In practice, for coupled quantum wires and wells in experimentally attainable regimes,  $D \gg 0$ , and usually  $\approx 1$ .<sup>4,5,21</sup>

As it is intuitive due to the weaker confinement, the binding energy of the 2D states is smaller with respect to 1D systems. In any case, even for 2D systems, not only the ground state, but also the first excited state energy is well reproduced within the variational model.

The accurate description of the energy behavior in the region far from  $D = 0$  does not necessarily imply *a priori* an accurate description of the eigenfunctions. The latter is important whenever response functions have to be computed, as the knowledge of the eigenstates is required, e.g., for the computation of transition matrix elements, in perturbation theory, etc.. Figure 3 shows the variational (solid) and the numerical (dashed) eigenfunctions, for the ground (black) and the first excited (red) states, at three different values for  $D$ , namely  $D = 0.5$  (left), 1 (center), and 2 (right). The top (bottom) row displays 1D (2D) results. In the 2D case, the slice of the wave functions at  $y = 0$  is displayed. Since  $\phi_{1y}(x, y = 0) = 0, \forall x$ , only  $\phi_{1x}(x, y = 0)$  is shown.

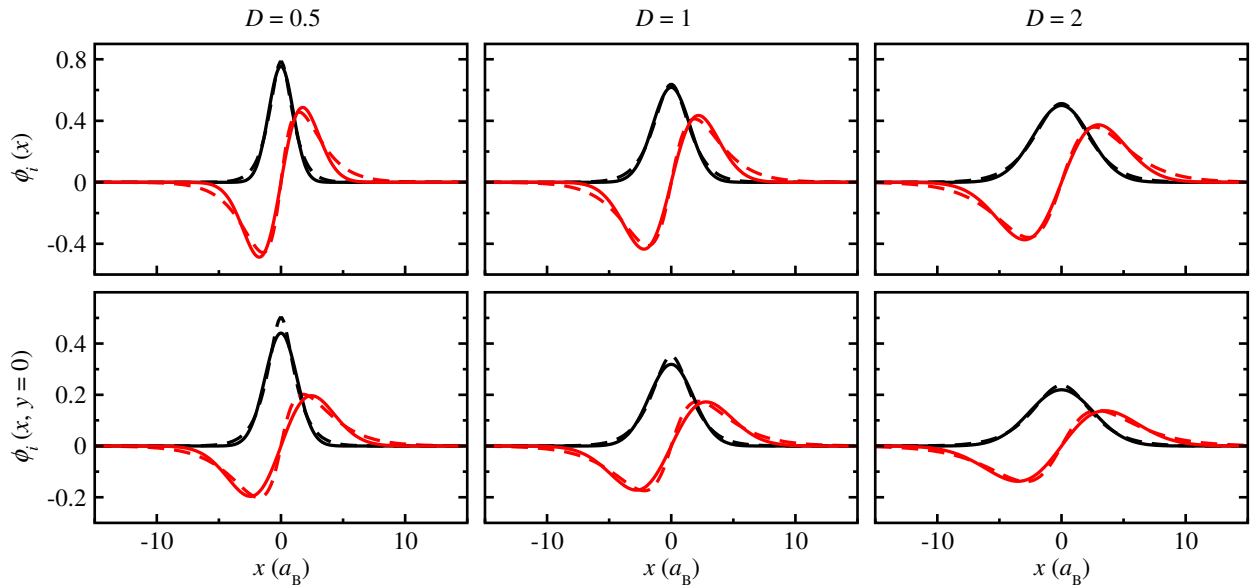


FIG. 3. Ground (black) and first excited (red) states for different bias distances  $D = 0.5$  (left), 1 (center), and 2 (right). Variational (solid), and numerical (dashed) wave functions. Top row: 1D system (coupled quantum wires); Bottom row: 2D system (coupled quantum wells), slice at  $y = 0$ .

Figure 3 exposes how the variational states are in good agreement with the numerically exact states in each of the cases presented here, which characterize a wide range of experimental regimes for coupled-quantum-wires and -wells systems. Note that, as  $D$  is increased, the eigenfunctions broaden, as it is natural due to the weaker Coulomb interaction.

## B. Results for GaAs-based heterostructures

We now specialize to the case of GaAs-based systems, widely adopted for the experimental realization of coupled quantum wires and wells poor in defects. As mentioned in the Introduction, these are the mostly exploited systems for the study and the propagation of Wannier-Mott spatially indirect excitons, which can be modeled in a hydrogen-like fashion,<sup>22</sup> the electron and the hole being separated thanks to an external electrostatic field, by a minimum bias distance  $d$  along the growth axis of the heterostructure. The distance  $d$  can be thought of as the center-to-center separation between the two wires (1D) or wells (2D), grown in an insulating AlGaAs matrix. We take typical GaAs parameters, namely  $\epsilon_r = 12.9$ , and a reduced effective mass  $m = (m_e^{-1} + m_h^{-1})^{-1} = 0.042 m_0$ , since  $m_e = 0.067 m_0$ , and  $m_h = 0.111 m_0$  are the electron and hole effective masses, respectively.<sup>17</sup>

In Fig. 4 we report the characteristic length parameters  $l_i$  (top), as well as the relative motion energy levels  $\varepsilon_i$  (bottom),  $i = 0, 1$ . We show the values from both exact numerical diagonalization and the variational method. The energies  $\varepsilon_i$  can be obtained by expressing the results of Sec. III A in terms of the effective Rydberg and Bohr radius for an electron-hole pair in GaAs, namely  $a_B = 16.34$  nm and  $\text{Ry} = 3.416$  meV. The separation  $d$  is varied from 10 to 20 nm, since this is the standard range of  $d$  in typical GaAs-based devices.<sup>4,21</sup>

## IV. CONCLUSIONS

We applied the variational method in 1D and 2D to obtain the ground and the first excited states for a Hamiltonian characterized by a soft-Coulomb potential  $V(r) \sim 1/\sqrt{r^2 + d^2}$ , dependent on the parameter  $d$ , which represents a bias distance. The first eigenstates of the quantum harmonic oscillator, chosen as trial functions, provide an accurate description of the exact eigenfunctions – which we have numerically computed via a finite-difference solver – whenever  $d$  is greater than a few tenths of the effective Bohr radius of the system; this is the typical condition in experimentally attainable regimes. The variational eigenenergies are in good agreement with their numerical equivalent, as well. All in all, the variational method provides a clear, analytical description of the physical problem related to the soft-Coulomb potential, at a very good level of accuracy, and within the typical background of undergraduate courses on quantum mechanics.

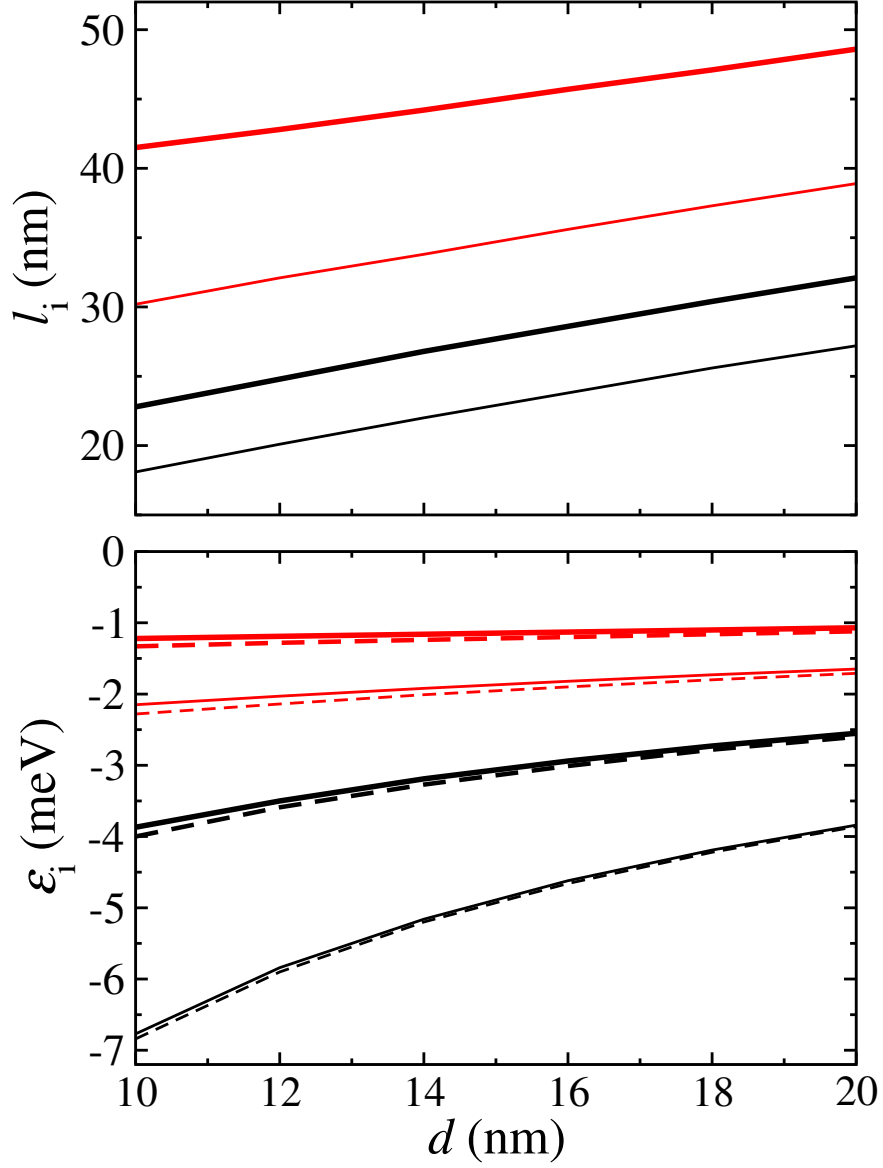


FIG. 4. Behavior of 1D (thin lines) and 2D (thick lines) system properties as a function of the distance  $d$  between the centers of two quantum wires and wells, respectively, for GaAs based devices. Legend as in Fig. 2.

## V. ACKNOWLEDGEMENTS

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- <sup>1</sup> G. Bastard, *Wave Mechanics Applied to Semiconductor Heterostructures*, (Wiley-Interscience, 1991), Chap. IV and references therein.
- <sup>2</sup> In these cases the Schrödinger-like equation determines the envelope function, i.e., the long wavelength part of the true wave function of the crystal. However, often in literature and for our purposes, we do not distinguish between envelope and wave function.
- <sup>3</sup> In the 1D case the ground state has a divergent energy.
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- <sup>13</sup> See the Supplementary Material at [URL will be inserted by AIP] for a Wolfram Mathematica code to obtain the optimal variational parameters and energies in 1D and 2D, after solving the related transcendent equations.
- <sup>14</sup> This comes from the definition  $U(1/2, 0, z) \equiv -\pi^{-1/2}e^{z/2}z[K_0(z/2) - K_1(z/2)]$ . [Reference at <http://functions.wolfram.com/07.33.03.0352.01>].
- <sup>15</sup> We exploit the definition  $U(3/2, 1, z) \equiv 2\pi^{-1/2}e^{z/2}[(z+1)K_0(z/2) - zK_1(z/2)]$ . [Reference at <http://functions.wolfram.com/07.33.03.0442.01>].
- <sup>16</sup> Wolfram Research, Inc. Mathematica 8.0.
- <sup>17</sup> It may be noteworthy to remark that the states  $\phi_i$  must be only considered as trial functions, independently of the fact they are solution of some harmonic oscillator (HO) problem: the HO eigenenergies  $E_i = (i + 1/2)\hbar\omega_i$ , where  $\omega_i \equiv \hbar/(ml_i^2)$ , with  $l_i \equiv \beta_i^{-1/2}$ , have no particular physical meaning for the soft-Coulomb problem here considered. In fact, within the variational method, the energies  $\varepsilon_i$  are defined as expectation values of the Hamiltonian on the states  $\phi_i$ , once the optimization is performed.
- <sup>18</sup> R. Lehoucq, D. Sorensen, and C. Yang, *ARPACK Users' Guide*, (Society for Industrial and Applied Mathematics, 1998).
- <sup>19</sup> R. Loudon, “One-Dimensional Hydrogen Atom,” *Am. J. Phys.* **27** (9), 649–655 (1959). In Loudon’s article some modified Coulomb potentials are also considered, like  $-1/(a + |x|)$ , where  $a$  is a positive constant, or a truncated Coulomb potential, where a cut-off  $x_0$  is introduced to form a well of depth  $-1/x_0$  for  $|x| < x_0$ .
- <sup>20</sup> G. Q. Hassoun, “One- and two-dimensional hydrogen atoms,” *Am. J. Phys.* **49** (2), 143–146 (1981).
- <sup>21</sup> G. J. Schinner, J. Repp, E. Schubert, A. K. Rai, D. Reuter, A. D. Wieck, A. O. Govorov, A. W. Holleitner, and J. P. Kotthaus, “Confinement and Interaction of Single Indirect Excitons in a Voltage-Controlled Trap Formed Inside Double InGaAs Quantum Wells,” *Phys. Rev. Lett.* **110** (12), 127403–[1–5] (2013).

<sup>22</sup> F. Grasselli, A. Bertoni, and G. Goldoni, “Exact two-body quantum dynamics of an electron–hole pair in semiconductor coupled quantum wells: a time dependent approach,” *Phys. Rev. B* **93** (19), 195310–[1–11] (2016).

<sup>23</sup> For the hole, whose mass tensor is characterized by a strong anisotropy in GaAs, we take the mass along the direction perpendicular to the growth direction of the heterostructure. See Ref. 22 for further details.