Variational method for calculating the binding energy of the base state of an impurity $D^-$ centered on a quantum dot of GaAs-Ga$_{1-x}$Al$_x$As

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Abstract. In quantum mechanics it is very difficult to obtain exact solutions, therefore, it is necessary to resort to tools and methods that facilitate the calculations of the solutions of these systems, one of these methods is the variational method that consists in proposing a wave function that depend on several parameters that are adjusted to get close to the exact solution. Authors in the past have performed calculations applying this method using exponential and Gaussian or orbital functions with linear and quadratic correlation factors. In this paper, a Gaussian function with a linear correlation factor is proposed, for the calculation of the binding energy of an impurity $D^-$ centered on a quantum dot of radius $r$, the Gaussian function is dependent on the radius of the quantum dot.

1. Introduction
Nowadays quantum mechanics is an area of physics with a very important boom, since its applications are very diverse, such as, for example, in microelectronics, optoelectronics and other areas where nanotechnology is present [1] and one of the highest concerns is the calculation of link energies, since it guarantees the stability of the quantum system. To study such systems and perform energy calculations, there are many models, methods and tools that allow to address the development of these complex systems, one of these methods is the variational method, where past research has shown the importance of correlation factors for solution of the Hamiltonian [2-5], ensuring the stability of the impurities, in this case, $D^-$ with a confining potential that can be a well or quantum point. In this particular work we seek to calculate the energy of the base state for an impurity $D^-$ centered on a quantum dot of GaAs / Ga$_{1-x}$Al$_x$As using as a wave function a Gaussian function as a function of the radius of the quantum dot, with a factor of linear correlation, which have shown their importance when performing calculations supported by the Monte Carlo and variational methods [6-8].

2. Methodology
In the subject of modern physics taught at the Universidad Pontificia Bolivariana based in Bucaramanga, (Santander, Colombia), one of the topics developed is that of quantum mechanics applied to the solid state, beginning by studying the matter waves, the wave duality particle and expected values until arriving at the Hamiltonian approach in one, two and three dimensions. In the class theoretical calculations of simple models are developed, such as the free particle, particle in a box, finite square well and quantum oscillator, but taking advantage of the fact that the university has an Advanced
Computation Center (ACC) they want to use these resources for the calculation of slightly more complex systems such as impurities $D^-$ centered on quantum dots GaAs / Ga$_1$-xAl$_x$As, for this students are formed under the direction of the teacher who teaches the subject in the programming language Fortran which is the chosen one for the realization of the calculations. The calculation that we want to perform is that of the link energy in this quantum system and for this, it is taken Hamiltonian to a hydrogen model, solving it through the variational method, and for this a Gaussian wave function is proposed that is radio dependent of the quantum dot but where a linear correlation factor is given importance, since in previous studies some authors have shown the importance of these factors to guarantee or ensure the stability of the quantum system [9].

In the work we propose the calculation of the bond energy in the base state of the impurity $D^-$ centered on a spherical quantum dot of radius $R$ of GaAs/Ga$_1$-xAl$_x$, where the wave function is a Gaussian in which takes into account the distances from the center of the quantum dot to the electrons present in the system.

The Hamiltonian for this system is of the form:

$$H = H(r_1) + H(r_2) + 2/r_{12}$$  \hspace{2cm} (1)

Where $r_{12}$ is the distance between the electrons and $r_1$ and $r_2$ are the distances of each electron to the nucleus. As can be seen, we have the sums of energies present in the quantum system, such as the kinetic and potential energies of the particles and the interaction between them, the Hamiltonian for each of the particles is:

$$H(r_1) = -\nabla^2_1 + V(r_1) - 2/r_1$$  \hspace{2cm} (2)

$$H(r_2) = -\nabla^2_2 + V(r_2) - 2/r_2$$  \hspace{2cm} (3)

Where $V(r)$ is the potential that limits the motion of the particle in two dimensions, and is defined as follows:

$$V = \begin{cases} 
0 & r < R \\
V_0 & r > R 
\end{cases}$$  \hspace{2cm} (4)

The proposed wave function as a function of variational parameters is of the form:

$$\psi(r_{12}, r_1, r_2, \theta) = \sum_{i=1}^{2n} A_i (1 + \delta_i r_{12}) e^{-\alpha_i r_1^2 - \beta_i r_2^2}$$  \hspace{2cm} (5)

Where $A_i, \delta_i, \alpha_i, \beta_i$ are the variational parameters that satisfy the cyclic conditions of symmetry:

$$A_{n+1} = A_1 = 1; \quad A_{n+i} = A_i; \quad \alpha_{n+i} = \alpha_i; \quad \beta_{n+i} = \beta_i; \quad \delta_{n+i} = \delta_i \quad i = 1, 2, 3, \ldots, n$$  \hspace{2cm} (6)

When we introduce the wave function into the Hamiltonian, five integrals appear that can be brought into the form of Gamma functions. These are integral energy and correspond to the term of overlap, kinetic energies of the electrons, potential in the barrier, Coulomb interaction with the nucleus and electrostatic repulsion between the electrons which are resolved in the ACC.

3. Results

The binding energies were calculated as a function of the radius of the quantum dot and concordance was observed with other works performed with linear and quadratic correlation factors with exponential wave functions.

It is observed in the data that the energy decreases when the radius of the quantum point increases and increases when it decreases [10]. This surprised the students, since in the analysis of the formula for other systems, such as a quantum well, the energy is inversely proportional to the width of the well, and
it would be expected that for very small widths the energy would continue to increase, but not what the experimental evidences and developed calculations show, something similar happens at the quantum point, it would be expected to continue increasing for very small radii, but the calculations show that the energy has a maximum for a critical radius of approximately 36Å and after this value decreases, this means that the energy changes drastically for values of r less than 36Å, this behaviour is due to the overflow of the wave function, this means that the radius of the quantum point of this value should not be decreased, since the system is affected.

### Table 1. Results of the link energy as a function of the radius of the quantum dot.

| R(Å) | Es(R) |
|------|-------|
| 1.9  | 0.067 |
| 31   | 2.245 |
| 42   | 2.143 |
| 60   | 1.865 |
| 65   | 1.814 |
| 70   | 1.782 |
| 99   | 1.241 |

### 4. Conclusions

The variational method, through history, has proved to be a very efficient method when calculating the link energies for a quantum system and in this particular case it was not the exception, and it was possible to calculate through this, the energy of link of the base state of an impurity $D^-$ centered on a quantum dot of GaAs-Ga1-xAlxAs and the results showed great agreement with other calculations made by other authors in the past.

The maximum energy value was obtained for a critical radius around 36Å, and after this value, the energy drops sharply.

It is observed from the results that for large radii of the quantum dot the binding energy is lower.

The importance of the correlation factors for the stability of the quantum system was evidenced since they take into account the distances and relationships between the particles.

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