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United Nations Educational Scientific and Cultural Organization
and
International Atomic Energy Agency
THE ABDUS SALAM INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

THE HYDROGEN ATOM BETWEEN TWO METALLIC MEDIA

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Abstract

We present calculations of the time of life and the displacements of the hydrogenic atomic levels in the vacuum between two metallic parallel surfaces. It is considered an approximation in which the electron interacts with the nucleus of infinite mass and with the two metallic media. In the vacuum the interaction is calculated with the method of electrostatic images. In the region near to the surfaces and inside the metal the approximations given by Borisov for the interaction of the electron with a Cu(111) surface [1] are used. The system is described with a non Hermitic Hamiltonian that is obtained on having applied the method of the transformations of dilatation [2]. Finally, the resultant Schrödinger equation is solved by means of the method of finite elements [9]. The presence of the second metallic medium gives place to an important decrease of the times of life in comparison to the case of the only surface reported in [1] and [10].

MIRAMARE – TRIESTE

November 2001

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1 The method of images in electrostatics

For a given set of boundary conditions, the solution to Laplace's equation is unique, so that if a solution $\phi(x, y, z)$ is obtained for any method, and if this ϕ it satisfies all the conditions in the border, then a complete solution of the problem has been found.
The method of images is a procedure to obtain this result without solving a differential equation, it is applied to the problem of one or more point charges in the presence of limiting surfaces, for example metallic, connected to ground or submitted to fixed potentials.
The idea of method of images consists of choosing a number of supplementary fictitious point charges, that together with the given charge, they create a field for which the surface of the given ideal conductor coincides with one of the equi-potential surfaces. If a charge e is given, this is obtained introducing a fictitious charge $\tilde{e} = -e$ placed in a point that represents the image reflected of the point e on the plane border of the conductive medium. In this way the new problem that arises is much simpler to solve, since the potential among punctual charges is given by Coulomb's law. The problem is reduced to find the set of images and their respective locations in the space.

2 A charge between two conducting media

Let's consider two infinite parallel conductive media enclosing a vacuum and a positive charge. We put on the charge the Z axis and in one of the plates another axis so that the intersection of these coincides with the origin of coordinates. The only coordinate that we are interested in is Z.
We call ℓ the separation between the planes and d the distance from our origin of coordinates to the point of location of the charge.
On having applied the method of images, taking into account that this method only is valid in regions far from both planes, we must consider the planes to be "mirrors" on which two images of the charge are formed, one for each plane. These two images have in turn, its own image, and so on; then the total number of images is infinite.

2.1 Position of the images

We divide the Z axis in a region 1 of (-∞, 0) and a region 2 of (0, ∞).
If we name:
Z_k^{1+}, the positive images in the region 1.
Z_k^{1-}, the negative images in the region 1.
Z_k^{2+}, the positive images in the region 2.
Z_k^{2-}, the negative images in the region 2.
One of the Z_k^2 is the original charge, the only charge that exists in the vacuum enclosed by both metallic regions.

We construct a succession of systems of charges that is an approximation to the system of infinite charges. With N a whole positive number:
For $N = 0$, the original negative charge.
For $N = 1$, initial (negative) charge with its two (positive) images.
For $N = 2$, previous ones plus other two negative images.
For $N = 3$, the previous ones plus other two positive images.
And so on.
The number of images in each case is $2N$. And the total number of charges, the real charge and all its images, is $2N + 1$. After, the total potential is divided by this quantity, in order to have the correct asymptotic limit for $\ell \to \infty$. For the case of a unique charge this interaction must tend to zero, and it is possible to think the problem as one of two charges with one of them equals to zero.
We have:
$Z_k^{1+} = -2k\ell - d,\ k = 0, 1, ..$
$Z_k^{1-} = -2k\ell + d,\ k = 1, 2, ...$
$Z_k^{2+} = 2k\ell - d,\ k = 1, 2, ...$
$Z_k^{2-} = 2k\ell + d,\ k = 0, 1, ...$
This can be unified to obtain the following result in both regions,

$$Z_k^{+} = 2k\ell - d, \tag{1}$$

for the position of the positive charges, with $k = 0, \pm 1, ...$ N_{even}: $k = -\frac{N}{2} + 1, ...\frac{N}{2}$. N_{odd}: $k = -\frac{N-1}{2}, ...\frac{N+1}{2}$.

$$Z_k^{-} = 2k\ell + d, \tag{2}$$

for the position of the negative charges, with $k = 0, \pm 1, ...$ N_{even}: $k = -\frac{N}{2}, ...\frac{N}{2}$. N_{odd}: $k = -\frac{N-1}{2}, ...\frac{N-1}{2}$.

2.2 Distance between the images

$$|Z_p^{+} - Z_n^{-}| = |2(p - n)\ell - 2d|,$$

here p is the position of the positive charges and n of the negative ones.

$$|Z_m^{+} - Z_j^{+}| = |2(m - j)\ell|.$$

We use this equation two times, one with m labeling positive charges, and then for negative charges. In both cases the j values start at $j = m + 1$, and $0 < d < \ell$.

2.3 Potential energy of interaction

Between positive and negative charges:

$$V_{pn} = \frac{-q^2}{|2(p - n)\ell - 2d|} \tag{3}$$

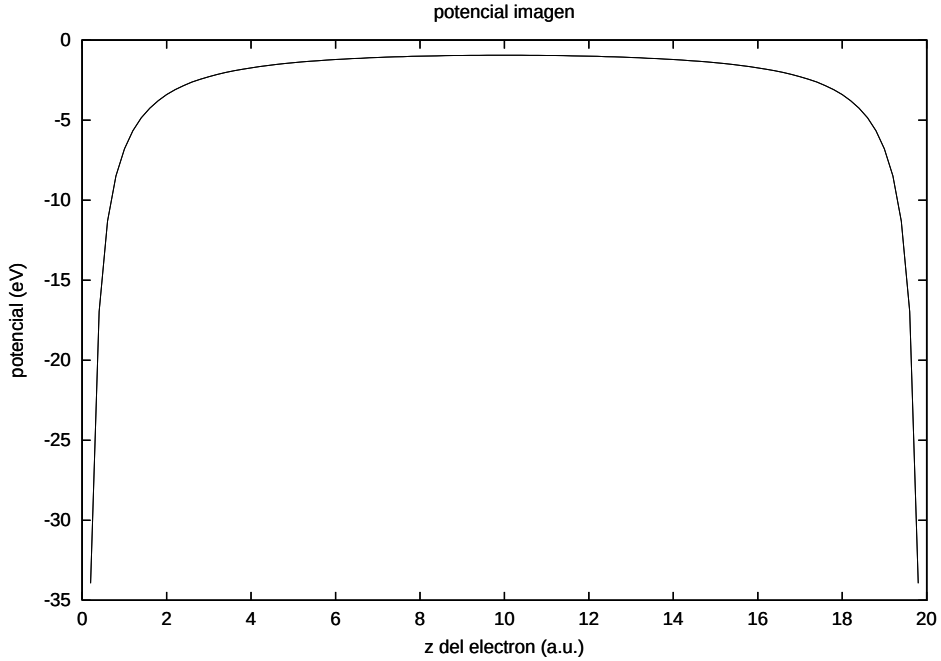

Figure 1: Potential energy of interaction of a negative charge with two metallic media, obtained by means of the method of electrostatic images.

Between charges of equal sign:

$$V_{pp} = V_{nn} = \frac{q^2}{|2(m-j)\ell|}, \tag{4}$$

where q is the magnitude of the real charge.

2.4 Total potential energy of interaction

$$V = \frac{1}{2N+1} \sum (V_{pp} + V_{pn} + V_{nn}) \tag{5}$$

Taking $\ell = 1$, then $0 < d < 1$, and assuming that the initial charge is not only negative but its value is 1, we have:

$$V = \frac{1}{(2N+1)} \sum \left[-\frac{1}{|2(p-n) - 2d|} + \frac{1}{|2(m^- - j^-)|} + \frac{1}{|2(m^+ - j^+)|} \right]. \tag{6}$$

It can be seen in Fig. 1 that in the region $0 < d < \ell$ V is negative and has only a maximum at $d = 0.5\ell$, and when $d = 0$ and $d = \ell$, V it tends to $-\infty$.

We conclude that for a charge in the middle of two conductive planes, the potential energy of interaction in the region included between both planes, is always attractive (it never becomes positive), it decreases infinitely when the charge approaches one of the planes and becomes maximum when the charge is exactly in the middle.

3 Two charges of opposite sign in the middle of two conductive planes

Applying the method of images and using the previous results we will find an expression for the potential energy of interaction in the region between the planes.
We will use cylindrical coordinates, (ρ, φ, Z), then the positions of the real charges are expressed by,
$q_{re}^{+} \Longrightarrow (0, 0, d_1)$, $q_{re}^{-} \Longrightarrow (\rho, \varphi, d)$.
For the initial negative charge we have the previous expressions for the positions Q^{+} and Q^{-} of the images, equations (2) and (3), for the Z coordinate.
For the initial positive charge:
$P^{+} = (0, 0, 2j\ell + d_1)$ (Position of the positive charges)
$P^{-} = (0, 0, 2m\ell - d_1)$ (Position of the negative charges),
where m, j change the same as in the previous development.

3.1 Distance between images

We will call distance on the same line, the distance between the images of a given charge. And crossed distance, the distance between the images of two charges.

3.1.1 Distances on the same line

$Q_p^{+} Q_n^{-} = |2(p-n)\ell - 2d|$. Positive-negative,
$Q_m^{+} Q_j^{+} = Q_m^{-} Q_j^{-} = |2(m-j)\ell|$. Positive-positive and negative-negative.
For the line that has real negative charge.
$P_p^{+} P_n^{-} = |2(n-p)\ell + 2d_1|$. Negative-positive,
$P_m^{+} P_j^{+} = P_m^{-} P_j^{-} = |2(j-m)\ell|$. Negative-negative and positive-positive,
for the line that has initial positive charge. With n, p, m, j changing of equal form that in the previous, case (see sections 2.1 and 2.2).

3.1.2 Crossed distances

Positive-Positive. $Q_k^{+} P_m^{+} = [\rho^2 + (2(m-k)\ell + d + d_1)^2]^{\frac{1}{2}}$.
Negative-Negative. $Q_m^{-} P_k^{-} = [\rho^2 + (2(k-m)\ell - d - d_1)^2]^{\frac{1}{2}}$.
N_{even}: $m = -\frac{N}{2}, .., \frac{N}{2}$. $k = -\frac{N}{2} + 1, .., \frac{N}{2}$ and N_{odd}: $m = -\frac{N-1}{2}, .., \frac{N-1}{2}$. $k = -\frac{N-1}{2}, .., \frac{N+1}{2}$.
Negative-Positive. $Q_m^{-} P_k^{+} = [\rho^2 + (2(m-k)\ell + d - d_1)^2]^{\frac{1}{2}}$,
N_{even}: $k, m = -\frac{N}{2} + 1, .., \frac{N}{2}$. N_{odd}: $k, m = -\frac{N-1}{2}, .., \frac{N+1}{2}$
Positive-Negative. $Q_m^{+} P_k^{-} = [\rho^2 + (2(m-k)\ell - d + d_1)^2]^{\frac{1}{2}}$,
N_{even}: $k, m = -\frac{N}{2}, .., \frac{N}{2}$ and N_{odd}: $k, m = -\frac{N-1}{2}, .., \frac{N-1}{2}$.

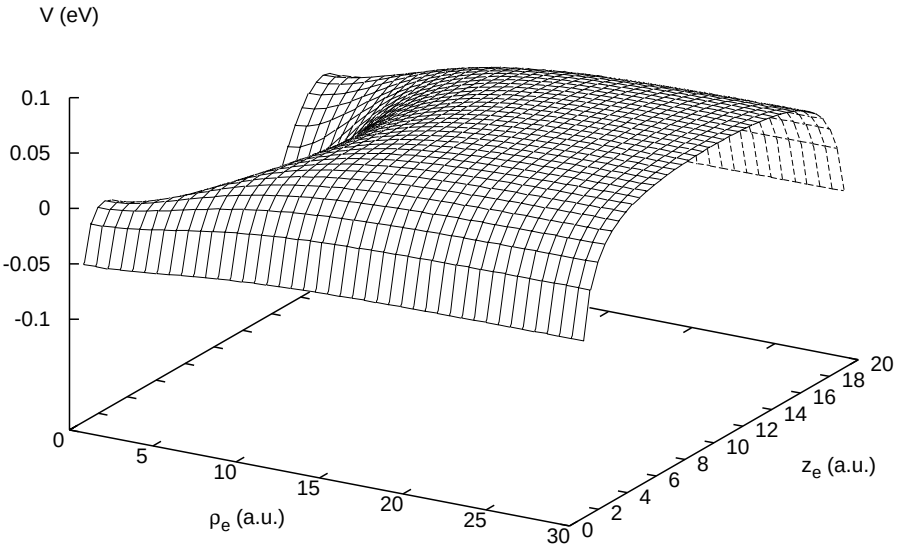

Figure 2: Surface of potential energy of interaction of a negative charge with two metallic media and with one positive charge placed between these, obtained by means of the method of the electrostatic images.

3.2 Potential energy of interaction

To simplify the obtained expressions we take: $\frac{q^-_{re}}{4\pi\epsilon_0} = -1$, $\frac{q^+_{re}}{4\pi\epsilon_0} = 1$ and $\rho = 1$ $\ell = 1$ then: $0 < d < \ell$ and $0 < d_1 < \ell$

$$
\begin{aligned}
V = & \frac{1}{2N+1}\sum \frac{1}{|2(m-j)|} + \frac{1}{|2(m_1-j_1)|} - \\
& \frac{1}{2N+1}\sum \frac{1}{|2(p-n)-2d|} + \\
& \frac{1}{2N+1}\sum \frac{1}{|2(j-m)|} + \frac{1}{|2(j_1-m_1)|} - \\
& \frac{1}{2N+1}\sum \frac{1}{|2(n-p)+2d_1|} + \\
& \frac{1}{2N+1}\sum \frac{1}{[1+(2(m-k)+d+d_1)^2]^{\frac{1}{2}}} + \\
& \frac{1}{2N+1}\sum \frac{1}{[1+(2(k-m)-d-d_1)^2]^{\frac{1}{2}}} - \\
& \frac{1}{2N+1}\sum \frac{1}{[1+(2(m-k)+d-d_1)^2]^{\frac{1}{2}}} - \\
& \frac{1}{2N+1}\sum \frac{1}{[1+(2(m-k)-d+d_1)^2]^{\frac{1}{2}}}
\end{aligned}
\tag{7}
$$

We are interested in the case the electron interacting with a nucleus of hydrogen and both

surfaces. Up to the moment only we have spoken about the region far from the two planes where it is valid the image method.

4 An electron near to the planes

In this region it is no valid to apply the method of images. Then we will use the following potential given by A. G Borisov *et al* [1].

$$V_{e-S}(z) = -\frac{V_0}{1 + Ae^{Bz}}, z_0 < z < 0, \tag{8}$$

$$V_{e-S}(z) = -\frac{1 - e^{-\lambda z}}{4z}, 0 < z < -z_0 \tag{9}$$

In [1] only one plate was considered, at the position $z = 0$, and these are the potentials for regions very near to the plate, with z_0 a negative number whose magnitude is very small.
(9) and (10) constitute the model of free electrons (or "jelly") for a metallic surface when $z_0 = 0$. It must be modified to reproduce the principal characteristics of the surface owed to the crystalline structure of the metal. In this way, the reference [1] proposes the following as model for Cu(111).
For the most internal region of the metal other two expressions are proposed, which modelates the crystalline structure:

$$V_{e-S}(z) = -V_0 - 0.5V_G\{1 - \cos[G(z - z_0)]\}, z_0 - \frac{\pi}{G} < z < z_0, \tag{10}$$

$$V_{e-S}(z) = -V_0 + V_G \cos[G(z - z_0)], z < z_0 - \frac{\pi}{G}. \tag{11}$$

For the region $z > z_0$ the potential is produced by the electron and its image.
For simplicity we will extend this model to the case of two metallic planes. This is valid if the presence of a metallic medium does not alter the properties of other one, which *a priori* is true only if the separation of both metallic regions is sufficiently big. Besides in (8)-(11) the modification of the interaction electron - surface caused by the presence of the nucleus is ignored, which is expected to be correct only if the separation nucleus - surface is sufficiently big.

4.1 A one-dimensional model

We have a plate at $z = 0$ and other one at $z = \ell$. Then the potential has the approximate form given by,

$$V_{e-S}(z) = -V_0 + V_G \cos[G(z - z_0)], z < z_0 - \frac{\pi}{G} \tag{12}$$

$$V_{e-S}(z) = -V_0 - 0.5V_G\{1 - \cos[G(z - z_0)]\}, z_0 - \frac{\pi}{G} < z < z_0 \tag{13}$$

$$V_{e-S}(z) = -\frac{C}{1+Ae^{Bz}}, z_0 < z < 0 \tag{14}$$

$$V_{e-S}(z) = -\frac{1-e^{-\lambda z}}{4z}, 0 < z < z_1. \tag{15}$$

For $z_1 < z < l - z_1$ we have the potential image given by (7). Where z_1 is introduced as a parameter that allows the continuity with the image potential.

$$V_{e-S}(z) = -\frac{1-e^{-\lambda(\ell-z)}}{4(\ell-z)}, \ell - z_1 < z < \ell \tag{16}$$

$$V_{e-S}(z) = -\frac{C}{1+Ae^{-B(z-\ell)}}, \ell < z < \ell - z_0 \tag{17}$$

$$V_{e-S}(z) = -V_0 - 0.5V_G\{1-\cos[G(z-\ell+z_0)]\}, \ell - z_0 < z < \frac{\pi}{G} + \ell - z_0 \tag{18}$$

$$V_{e-S}(z) = -V_0 + V_G\cos[G(z-\ell+z_0)], z > \frac{\pi}{G} + \ell - z_0 \tag{19}$$

4.2 Expression for the potential of interaction of an electron with a nucleus and the two metallic regions

For this case we have the same expressions given by the equations (12) to (19), except that in the region $z_1 < z < \ell - z_1$ we consider a potential image given by the equation (8).

We take the origin of coordinates at the left surface. The problem was solved in a region whose z coordinate is located between $-29a.u$ and 49 a.u. approximately. We take $\ell = 20$ a.u. and locate the nucleus in the half of both surfaces, that is at 10 a.u. The values of other parameters were taken from [1]:
$\lambda = 1.5a_0^{-1}$, $V_0 = 11.61$ eV, $G = 1.596a_0^{-1}$, $V_G = 2.55$ eV, $Z_0 = -2.0106a_0$, with $a_0 = 1.0$ a.u. For Z_1 we take a value of 1 a.u., and it was chosen from the graphs of (8) and (16), looking for an approximate point of intersection. The values of A and B are determined by applying continuity conditions of (15) and (16) for the functions and their derivatives, and they are:
$A = 4V_0/(K\lambda) - 1 = 0.1377$ dimensionless.
$B = (1+A)^2K\lambda^2/(8AV_0) = 6.1964(a.u)^{-1}$. $K = 27.21183$ eV, it is a factor that appears in (16) for dimension reasons, since all the potentials are given in eV. The parameter C is defined to have continuity of (14) and (15) at the point Z_0, that is: $C/(1+Ae^{BZ_0}) = V_0$, but $1 + Ae^{BZ_0}$ is approximately 1, therefore C is practically V_0.
We observe in figure 3 the form of the one-dimensional potential. With the nucleus in the middle of the plates, that are separated 20 a.u. The movement of the electron is only along the Z axis. We are going to concentrate on the solution of this case, the solution to Schrödinger's equation with the one-dimensional potential described in the previous lines.

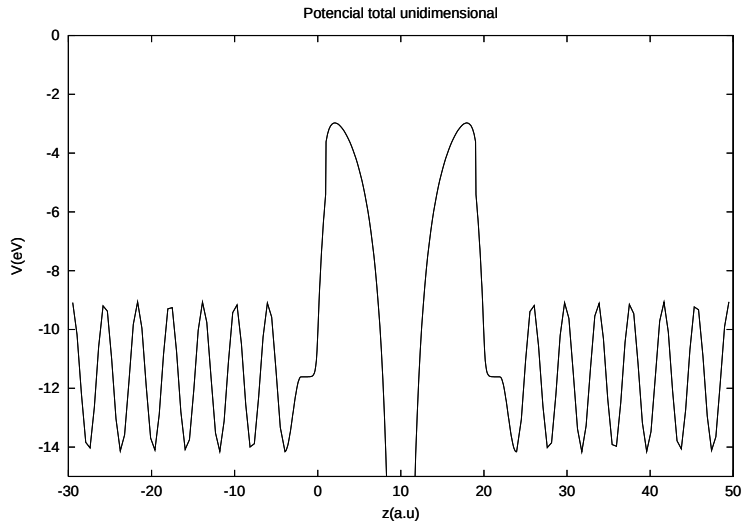

Figure 3: Potential energy of interaction of a negative charge with two Cu(111) surfaces and a positive charge.

4.3 Bands of energy of H between two metallic surfaces

The energy spectrum of this system is continuous. If the Schrödinger equation (20) is written in a matrix form, by expanding the wave function into a finite basis set, the continuous spectrum is approximated by a finite series of discrete eigenvalues. The overall set of energy eigenvalues will manifest itself with subsets of clustered eigenvalues, which could mimic a band structure of continuous eigenvalues.

We solved numerically the Schrödinger equation with the potential energy $V(z)$ previously found. The problem has cylindric symmetry and the states can be classified according to the projection of angular momentum on the Z axis, m. This gives rise to a partial differential equation in the variables (ρ, z).

The finite element method was used to solve the 2-dimensional partial differential equation. The general details of the method can be found elsewhere, e.g. in [9]. For this case, a mesh of 900 squares was formed into a square region whose side was 81.1 au. The metallic regions had a wide of 30.55 a.u. and enclosed a vacuum of wide 20 a.u. The nucleus was put in the center. The wave function was expanded in a local basis formed by Hermite interpolation polynomials of fourth degree, defined by 3 local nodes and 1 degree of freedom (see [5]). Thus, the problem was reduced to solve a generalized eigenvalue problem involving 3721×3721 Hermitic matrices.

This procedure allows us to find the band energy structure and the eigenfunctions. The results are shown in figure 4

Also the method gives the wave functions. Figure 5 shows the wave functions corresponding to the first energies of the band starting at -11496.96 eV. We can see that the electron rapidly becomes unlocalized when the excitation increases. Note that electron wave function spreads into the horizontal direction, but becomes localized in the vertical direction Z, for the shown states.

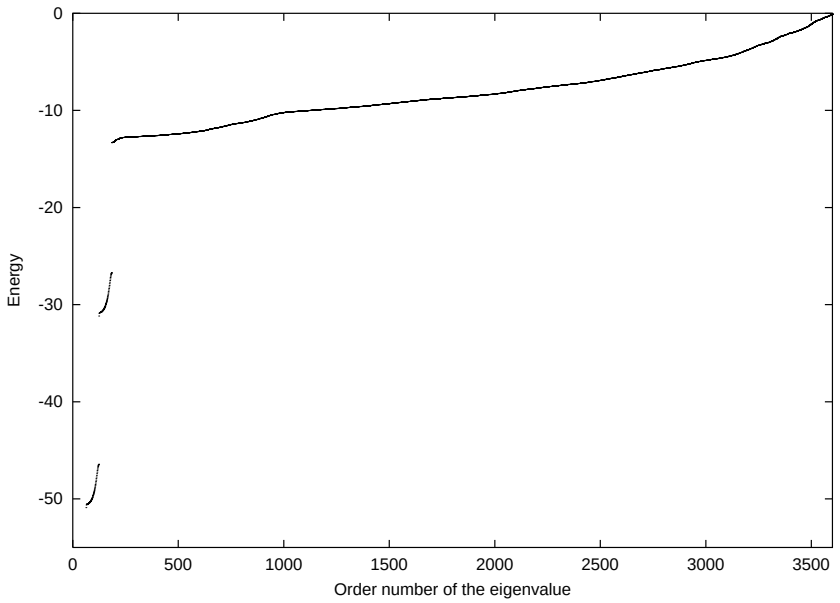

Figure 4: Structure of the energy bands of the electron interacting with the nucleus and two metallic surfaces. For clarity reasons a deep band of energy levels in the interval [-11496.96,-11492.00] eV is omitted.

5 The method of dilatation transformations

In the article cited in the previous section, [3], is studied the movement of the electron in a potential $V(z)$, using the wave packet propagation method (WPP). In this work will be used an alternative method, called dilatation transformation method [4].

5.1 Resonant states

The movement of an electron under the potential $V(z)$ has no bound states when the distance ℓ is tiny, admitting however quasi-bound states or resonances, the other states are in the continuum and are grouped in bands. This is due to the potential in the vacuum region acts as perturbation of the potential in the metallic medium that, as it is known, gives rise to a energy band electronic structure.

The goal is to identify in the set of solutions of

$$\left[-\frac{\hbar^2}{2m}\bigtriangledown^2 + V(z)\right]\Psi(\vec{r}) = \frac{\hbar^2 k^2}{2m}\Psi(\vec{r}), \tag{20}$$

those that possess $\vec{k}$ of complex magnitude

$$z_r = k_r + i\beta_r, \tag{21}$$

and complex energy

$$E_r = e_r - \frac{i}{2\tau}, \tag{22}$$

where

$$e_r = \frac{\hbar^2}{2m}(k_r^2 - \beta_r^2)$$

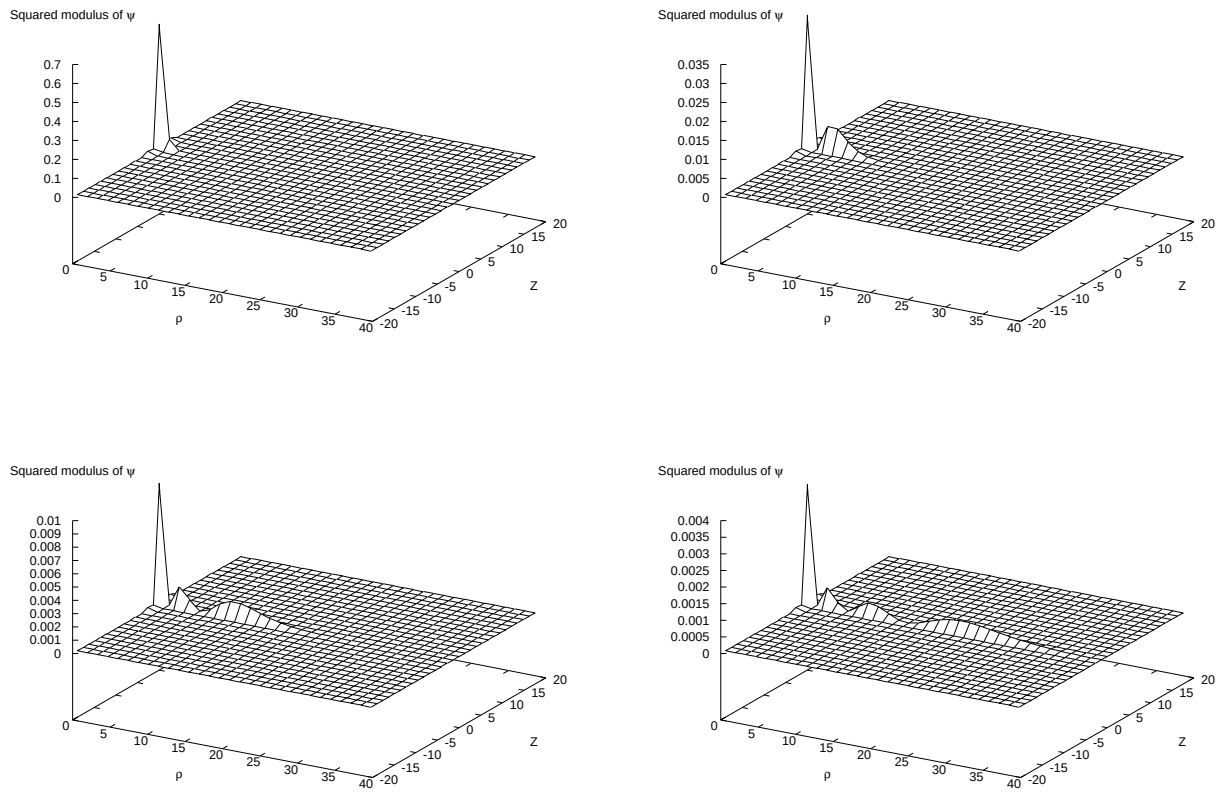

Figure 5: Module squared of the wave functions corresponding to the first 4 eigenvalues of the band starting at -11496.96 eV.

$$\frac{1}{2\tau} = \frac{-\hbar k_r \beta_r}{m}.$$

These states exponentially decay in time if $\beta_r < 0$.

In the dilatation transformation method the solutions of the complexified Schrödinger equation are analyzed. In this way the resonances appear like a type of solutions of this equation. The transformation of all the variables of position of the problem is carried out thus, $r \to re^{i\theta}$.

$\mathcal{R}(\theta)$ is a rotation angle and $e^{-\mathcal{I}(\theta)}$ is a scale factor in the dimensions of the problem. This does that the Hamiltonian $\widehat{H} = \widehat{T} + \widehat{V}$ now depends on θ as a parameter,

$$\widehat{H}(\theta) = e^{-2i\theta}\widehat{T} + e^{-i\theta}\widehat{V} \tag{23}$$

When the interactions are Coulombic, the solutions of the Schrödinger equation, $E_n(\theta)$ and $\Psi_n(\theta)$ will depend on θ:

$$[\widehat{H}(\theta) - E_n(\theta)]\Psi_n(\theta) = 0. \tag{24}$$

Balslev and Combes [6] show mathematically that:
(i) The bound states of $\widehat{H}(\theta)$ have eigenvalues that remain fixed at their real values without depending on θ.

(ii) If the system possesses different ionization thresholds, such that they extend toward the continuum, then these energies rotate an angle $-2\mathcal{R}(\theta)$ in the lower complex half-plane.
(iii) When $\mathcal{R}(\theta)$ enlarges and one of the lines of energy of the continuum crosses a resonance pole, a new eigenvalue of $\widehat{H}(\theta)$ appears at the position of the said resonance.
(iv) When appears a resonance eigenvalue, it remains invariant with θ until be covered by another branch for a value θ_0 in which the resonance disappears.

An advantage of the method of dilatation transformations is that Schrödinger equation is solved using the same methods of solution that in bound state problems. It is usual to convert the differential equation into a matrix one and to diagonalize the Hamiltonian matrix. As $\widehat{H}(\theta)$ is complex a non Hermitic matrix is obtained, whose eigenvalues will be complex.

5.2 Stability criterion

Yaris and Winkler [4] present an analytic criterion that permits to choose a value of θ. Theoretically the solution does not depend on θ, the numerical errors give rise that the eigenvalues change when θ changes. Then it is necessary to find an optimum value of θ. No minimization criterion is utilized here, despite that it is used in the variational methods.

If $\theta = \alpha + i\beta$ and the following complex function is defined,

$$R(\alpha, \beta) = \frac{E_r(\alpha, \beta)}{< \widehat{T}(\alpha, \beta) >_R},$$

then the optimum value of θ is such that $R(\alpha, \beta)$ is the most nearby to the point of the complex plane $(-1, 0)$. In theory $R(\alpha, \beta) = -1$ at the state of resonance. $< \widehat{T}(\alpha, \beta) >_R$ is the average value of the kinetic energy at the resonant state $\Psi(\alpha, \beta)$.

5.3 Resonant states of H between two metallic surfaces

Mathematically the problem consists of solving Schrödinger's equation for an electron in interaction with a nucleus with potential energy $-1/r$ and with the metallic surfaces across $V_{e-S}(z)$. The dilatation transformations method is used to describe the resonances [4]. The Schrödinger's equation is solved using the method of finite linear elements [5].
The Hamiltonian of the problem in cylindrical coordinates is:

$$\widehat{H} = \frac{\widehat{P}_\rho^2}{2} + \frac{\widehat{L}_z^2}{2\rho^2} + \frac{\widehat{P}_z^2}{2} - \frac{1}{r} + V_{e-S}(z) \tag{25}$$

where V_{e-S} is given by the equations in section 4.2. We use atomic units and cylindrical coordinate (ρ, ϕ, z) for the position of the electron, the nucleus is at the point $(0, 0, d)$ and the origin of coordinates is at the surface of the left side.

Due to the cylindrical symmetry the Z component of the angular moment of the electron is conserved and the movement in ϕ separates from the movement in the plane (ρ, z). For simplicity, in the present work we will analyze the case $\widehat{L}_z = 0$, $\widehat{P_\rho} = 0$. In this case it is

$\mathcal{R}$	$\mathcal{I}$
-18816.2	32402.2
-2678.61	4446.26
-1952.51	3111.68
-155.529	262.254
-155.529	262.254
-155.318	258.343
-155.318	258.342
-154.702	253.167
-154.717	253.14
-32.6285	24.3768
-32.6337	24.2476
-15.9907	7.9949
-15.9858	7.95648
-12.3156	4.02324
-12.3046	4.02034

$\mathcal{R}$	$\mathcal{I}$
-10.6442	1.92187
-10.6364	1.92149
-9.2675	0.0217606
-9.2593	0.023397
-8.38057	1.3413
-8.37298	1.34391
-7.01315	1.88747
-7.01041	1.8881
-5.82772	2.26913
-5.82744	2.26848
-5.82744	2.26848
-3.34365	2.52598
-3.34354	2.52587
-2.14609	2.53945
-2.14601	2.5394

Table 1: Some complex eigenvalues.

sufficient to solve the problem of the vertical movement of the electron, along the Z axis. There is known that the free one-dimensional H atom has the ground state with energy $-\infty$ and wave function type Dirac's delta [8]. This characteristic will demonstrate in the present problem.

Wave functions and eigenvalues of resonant states:

For the first result was not considered the criterion of stability of section 5.2, and a value of $\theta = \frac{2\pi}{6} = \frac{\pi}{3}$ was taken.

In table 1 the real and imaginary parts of the eigenvalues of the resonant states are shown.

We can observe that the series of energy values beginning at $-15.99eV$ accumulate at $-2.1eV$, as is to be expected according the graph of the potential in section 4.2.

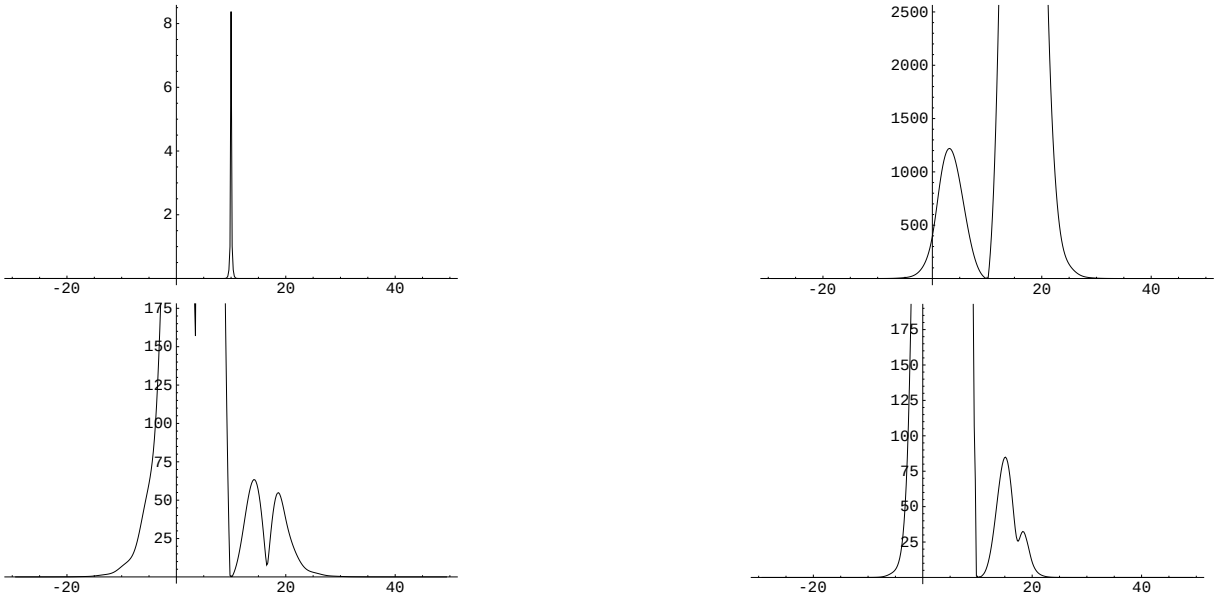

Figure 6: Module squared of the wave functions corresponding to the eigenvalues (a) $-18816.2 + 32402i$, (b) $-155.529 - 262.254i$, (c) $-155.318 - 258.342i$ and (d) $-3.34354 + 2.52598i$.

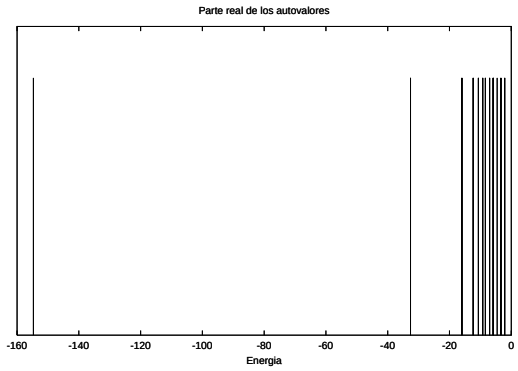

Figure 7: Position of some of the resonances of the electron.

Conclusions

A model for the potential energy of interaction of an electron with a nucleus and two metallic media was presented. A first approximation to the problem was obtained taking the nucleus of infinite mass and supposing that the interaction with one of the metallic materials is not modified by the presence of the nucleus nor the second medium. An additional approach consisted of considering only the one-dimensional movement of the electron in perpendicular direction of the conducting planes.

It was found that the method of the images allows to construct a succession of potentials that approximate to the real potential of interaction with the metallic media with an arbitrary exactitude. With the help of results found in the literature a potential valid in all the space was generated.

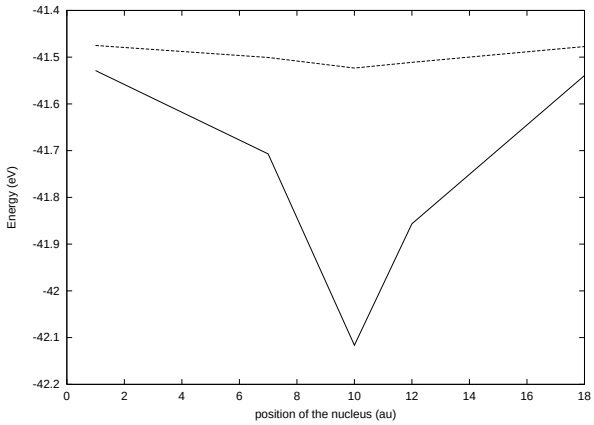

Figure 8: Energy of the first two eigenvalues as a function of the nucleus position. A minimum is reached when the nucleus is exactly in the middle.

With basis on this potential the method of the complex factor of scale was used to calculate the time of life and the displacements of the hydrogenoid atomic levels in the vacuum between two parallel metallic surfaces. It was verified that an advantage of this method is that the Schrödinger equation is solved using the same methods of solution that in problems of bound states.

In order to numerically solve the resulting complex eigenvalue problem, the finite element algorithm was used. An extension of the method consists on maintaining the indicated approaches but to consider the two-dimensional movement of the electron, in which we work at the moment. Other approaches such those of the Echenique and collaborators [7] are to be examined. Physically can be considered that the empty space included between both metallic media and the presence of the nucleus constitutes a disturbance that breaks the translation symmetry. Due to this, in addition to bands of energy, similar to the Bloch bands of a periodic potential, the resonant states appear.

The wave functions and the eigenvalues of the resonant states of lower energy states were found, for the one-dimensional model. These complex eigenvalues contain information on the location in energy of the corresponding resonances and their wide (from which the times of life are calculated). It is observed that the real parts of the energies form a succession that is accumulated in near values -2.1 eV.

Acknowledgements

Very constructive comments from Jean-Pierre Gauyacq, University of Paris South, Laboratory of Atomic and Molecular Collisions, Orsay, France, and Pedro Echenique, Department of Physics of Materials, San Sebastian, Spain, are gratefully acknowledged. We are pleased to acknowledge the Research Committee of the University of Antioquia (CODI), Medellín, Colombia for the financial support of the present work. JM has participated in this work within the framework of the Associateship Scheme of the Abdus Salam International Centre for Theoretical Physics,

Trieste, Italy.

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