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Tunneling Calculation in the Field Ion Microscope

Cálculo de Tunelamento com o Microscópio de Campo de Íon

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In this work we describe calculations of tunneling rate constants for the Field Ion Microscope (FIM) using one-dimensional model potential that simulates the ionization process in a FIM. We obtain expressions for the ionization rate constant (ionization probability per unit of time) of inert gas atoms as a function of their position above the surface. In order to calculate the probability of barrier penetration we have used the semiclassical (JWKB) approximation. We have also calculated ionization zone widths as the distance between points where ionization rate is a maximum and half of this value. An application to helium as the imaging gas is presented to highlight the power of the method.

Keywords: Tunneling; Field Ion Microscope; Barrier Penetration; JWKB Approximation.

Neste trabalho, descrevemos os cálculos realizados para as constantes de taxa de tunelamento para o Microscópio de Campo de Ion (FIM) usando um potencial modelo unidimensional que simula o processo de ionização em um FIM. Obtemos expressões para a constante de taxa de ionização (a probabilidade de ionização por unidade de tempo) de um gás de átomos inertes como uma função de suas posições acima da superfície. A fim de calcular a probabilidade da penetração de barreira, utilizamos a aproximação semiclássica (JWKB). Calculamos também as larguras das zonas de ionização com a distância entre os pontos onde a taxa de ionização é máxima e metade desse valor. Uma aplicação para o hélio como gás de imagem é apresentada para destacar o alcance do método.

Palavras-chaves: Tunelamento; Microscópio de Campo de Ion; Penetração de Barreira; Aproximação JWKB.

I. INTRODUCTION

The ionization of an atom by tunnel effect in a strong electric field is called field ionization. The high electric field necessary for this effect to be of practical interest became feasible following the invention of the field ion microscope (FIM) by E.W. Müller and co-workers [1, 2]. Nowadays, one of the most important applications of the FIM is the characterization of tips for use in the Scanning Probe Microscopy (SPM).

The FIM is a type of microscope capable of imaging individual atom at a surface of a sharp metal tip. In this device a sharp metal tip is placed in an ultra high vacuum chamber, which is backfilled with an imaging gas atoms, normally inert gas atoms such as helium. For field sufficiently high, these image gas atoms are field ionized by a quantum-mechanical tunneling process. The positively charged ions formed by this process are then accelerated by the electric field towards a screen, where they form an image. Tunneling into the metal surface is forbidden when the atom is closer to the metal surface than a critical distance be-

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cause the atomic-ionization level falls below the Fermi level of the metal and there are no empty states for one electron [4]. Beyond the critical distance there was a rapid decrease in tunneling rate. Then, most of the ionization occurs in an ionization zone close above the so-called critical surface, which is typically few angstroms above the emitter's metal surface.

In this work we calculate the ionization rate constant (ionization probability per unit of time) as a function of the applied field (we assume a uniform field) and the atom's distance from the metal surface. We utilize one-dimensional model potential which is chosen to yield a reasonable physical representation of the real system. We can use one-dimensional models because the tunneling is maximal in the direction normal to the metal surface. The ionization rate is not directly measurable physical quantity. However, a narrow ionization zone was observed as a narrow peak in the ion energy distribution [5] corresponding to a zone width of about $0,2$ Å. From our theoretical results we calculate ionization zone width. Throughout this paper we work in atomic units where $\hbar = m = e = 1$.

In a one-dimensional model, the ionization rate I is given by,

$$I = \nu P, \tag{1}$$

where ν represent the oscillating frequency about the nucleus, striking a potential barrier which it may penetrate and P is the probability of barrier penetration at one attempt by the electron to escape which is given in the JWKB approximation by (in atomic units)

$$P = \exp\left[-2^{3/2}\int_a^b \sqrt{V(x) - E}\, dx\right], \tag{2}$$

where $V(x)$ is the one-dimensional model potential, E is the total energy of the electron and a e b are the classical turning points, i.e. the zeros of $V(x) - E$.

We choose the model potential that is a good representation of the real system, but at the same time allowing analytical calculation of the electron-tunneling rate-constant. In a previous work we present a simple model calculation of the barrier penetration probability [6].

In this paper we will adopt the following model for potential energy. Inside the metal we considered a uniform depth potential well with sides of height ϕ above the Fermi level, where ϕ is the zero field work function of the metal. The atom is represented by a hydrogenic potential $-Z_{ef}/x$ centered of the nucleus of the atom and a uniform electric field is added. That is

$$V(x) = \begin{cases} -\phi, & \text{inside the metal} \\ -\frac{Z_{ef}}{x} - Fx, & \text{outside the metal} \end{cases} \tag{3}$$

where F is the magnitude of the electric field, Z_{ef} is a parameter to account for other effects like the potential from the positive ion and the image potentials the effective charge of the gas atom and x is measured from the nucleus of the atom (Figure 1).

The probability of barrier penetration is given by

$$P = \exp\left[-2^{3/2}\int_a^{z_0} \sqrt{B - Z_{ef}/x - Fx}\, dx\right], \tag{4}$$

where B is the binding energy of the gas atom and z_0 is the distance of the gas atom from the surface.

The integral above is not trivial. However, we can write

$$L = \int_a^{z_0} \sqrt{\frac{F\,(x_2 - x)\,(x - x_1)}{x}} dx, \tag{5}$$

where

$$x_1 + x_2 = \frac{B}{F}, \tag{6}$$

and

$$x_1 x_2 = \frac{Z_{ef}}{F}. \tag{7}$$

The integral (5) is tabulated by Gradshteyn and Ryzhik [7] and results

$$L = (F^{\frac{1}{2}})\left(\frac{2}{3}\sqrt{z_0}\left[\frac{B}{F}E(p) - \frac{2Z_{ef}}{B}K(p)\right]\right), \tag{8}$$

where $p^2 = (x_2 - x_1)/x_1$ and $E(p)$ and $K(p)$ are complete elliptic integrals that can be developed in series [7]

$$E(p') = 1 + \frac{1}{2}\left[\ln\left(\frac{4}{p'}\right) - \frac{1}{2}\right] p'^2 + \ldots \quad (9)$$

$$K(p') = \ln\left(\frac{4}{p'}\right) + \left[\ln\left(\frac{4}{p'}\right) - 1\right]\frac{p'}{4} + \ldots (10)$$

where

$$p' = \sqrt{1 - p^2} = \left(\frac{Z_{ef}}{Bz_0}\right)^{\frac{1}{2}}. \quad (11)$$

Substituting (9) and (10) into (8) we obtain:

$$L = \frac{2Bz_0^{(1/2)}}{3F^{(1/2)}} - \frac{Z_{ef}}{6F^{(1/2)}z_0^{(1/2)}} + \left(\frac{Z_{ef}}{3F^{(1/2)}z_0^{(1/2)}} - \frac{4F^{(1/2)}z_0^{(1/2)}Z_{ef}}{3B}\right)\ln\left(\frac{4B^{(1/2)}z_0^{(1/2)}}{Z_{ef}^{(1/2)}}\right). \quad (12)$$

The probability of barrier penetration is then given by

$$P = \left(\frac{4B^{(1/2)}z_0^{(1/2)}}{Z_{ef}}\right)^{\left(-\frac{2^{(3/2)}Z_{ef}}{3F^{(1/2)}z_0^{(1/2)}}\right)} \exp\left(-\frac{2^{(5/2)}Bz_0^{(1/2)}}{3F^{(1/2)}} + \frac{2^{(3/2)}Z_{ef}}{6F^{(1/2)}z_0^{(1/2)}}\right). \quad (13)$$

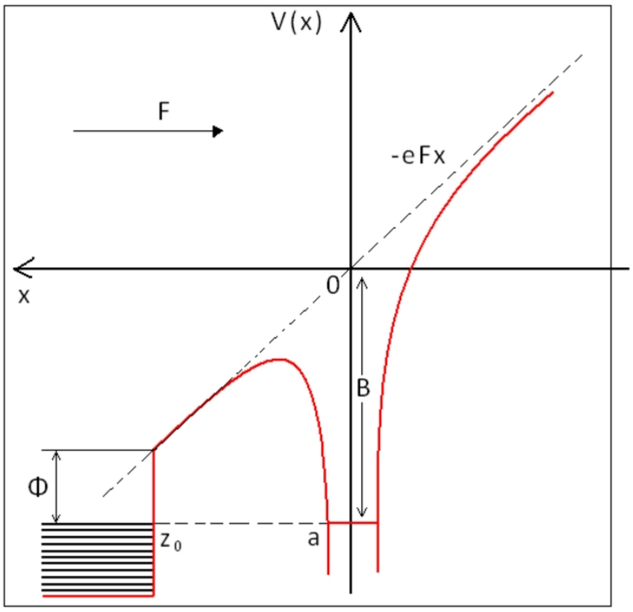

FIGURE 1: Model potential used in the tunneling calculation. B is the zero field ionization potential of the atom, a is the inner classical turning point and z_0 is the distance of the gas atom from the surface

II. EXPRESSION FOR THE TUNNELING RATE CONSTANT

We can now calculate the ionization rate. Field ionization is forbidden when the gas atom is closer to the metal surface than a critical distance z_c because otherwise the atomic ionization level falls below the Fermi level of the metal and there are no empty states for the electron to tunnel into [2]. This condition can be approximately expressed as

$$z_c = \frac{B - \phi}{F}. \quad (14)$$

For helium, $B = 25,4\ eV$ (0,93 u.a). In its ionization field of 45 V/nm (0.09 u.a) above a tungsten surface $\phi = 4,5\ eV$ (0,16 u.a), we find for the critical distance $z_c \simeq 4,4\ \mathring{A}$. Thus the Eq.(13) apply only when the atom is at a distance greater than z_c from the metal surface because $P = 0$ for $z_0 < z_c$.

On the other hand, for distances z greater than B/F (the outer classical turning point) the ionization rate become to the uniform field form. Thus we have the following expression for the ionization rate

$$
I(z_0) = \begin{cases} 0, \text{ if } \quad z_0 < z_c, \\ \\ \nu\left(\frac{4B^{(1/2)} z_0^{(1/2)}}{Z_{ef}}\right)^{\left(-\frac{2^{(3/2)} Z_{ef}}{3F^{(1/2)} z_0^{(1/2)}}\right)} \exp\left(-\frac{2^{(5/2)} B z_0^{(1/2)}}{3F^{(1/2)}} + \frac{2^{(3/2)} Z_{ef}}{6F^{(1/2)} z_0^{(1/2)}}\right), \text{ if } \quad z_c < z_0 < B/F, \\ \\ \nu\left(\frac{4B}{Z_{ef} F^{(1/2)}}\right)^{\left(-\frac{2^{(3/2)} Z_{ef}}{3B^{(1/2)}}\right)} \exp\left(-\frac{2^{(5/2)} B^{(3/2)}}{3F} + \frac{2^{(3/2)} Z_{ef}}{6B^{(1/2)}}\right), \text{ if } \quad z_0 > B/F. \end{cases} \tag{15}
$$

The Eq.(15) given the expressions for the tunneling rate-constant against the distance z of the gas atom from the metal surface.

In Figure 1 we plot the Eq.(15). We have used the values $B = 25,4\ eV$ $(0,93ua)$, $Z_{ef} = 1,5$ and $F = 45V/nm$ $(0,09ua)$. The frequency ν is calculated using a Bohr orbit model. For the helium we have [2] $\nu = 2,4 \times 10^{16}\ s^{-1}$ $(0,58ua)$.

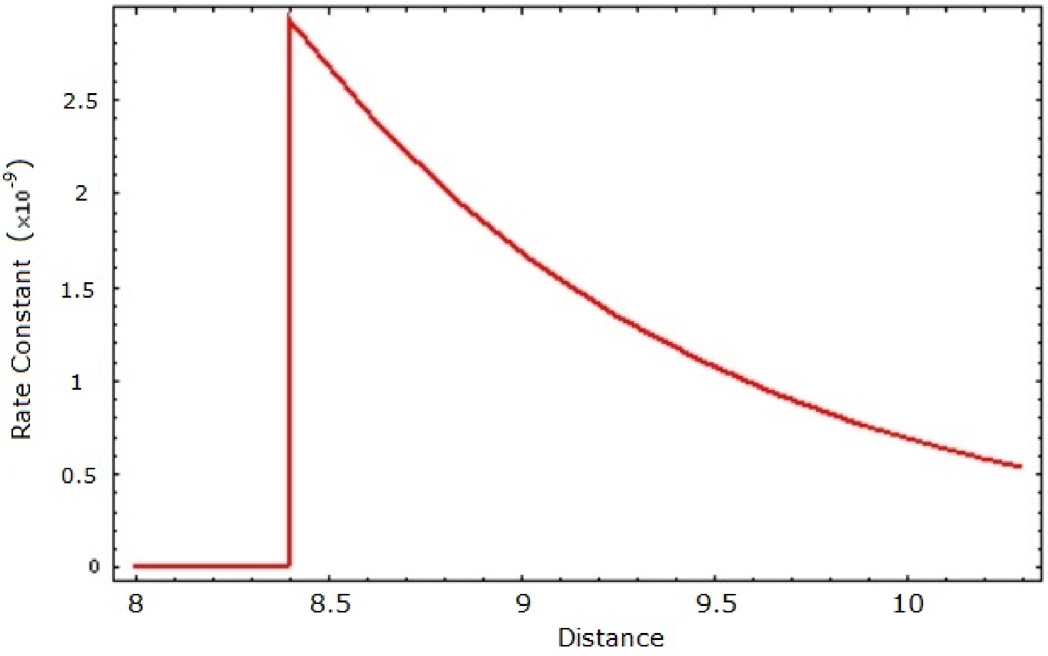

FIGURE 2: The tunneling rate constant versus the distance of a He atom from the metal surface with $F = 45V/nm$, $\Phi = 4.5eV$ $Z_{ef} = 1.5$.

The ionization rate, despite its enormous importance in understanding the process of field ionization is not a directly measurable physical quantity. As we saw, most of the ionization of the imaging atoms occurs in an ionization zone close above the so-called *critical surface*, which is at distances a few angstroms from the surface metal. This position can be inferred from the energy deficit of the ions on arrival at the screen, compared with the energy that they would have for the full potential difference between sample and screen.

In other words, if the ions is created in space at some distance from the surface, it will acquire less kinetic energy if it is created at the tip surface. As a consequence, the ionization distribution curves as a function of the energy deficit will indicate the position at which the ions are formed, and the width of this distribution will reflect the spatial extent of the ionization region above the metal surface.

The energy distribution of ionized gas atoms was first measured by Inghram and Gomer [4]. Soon after, Müller and Bahadur [8] measured the width of the energy distribution for imaging with argon and they found $\approx 2\ eV$. This implies that the width of the ionization zone is about $\approx 0.5\ \mathring{A}$. Later, the energy distribution of ions obtained by field ionization of He and another imaging atoms near the surface of a tungsten emitter was measured by Tsong and Müller [5]. They found for the half-width of the distribution an value between 0.5 and 0.7 eV. This corresponds to an ionization zone of 0.2 $\mathring{A}$.

To calculate the width of the ionization zone we can define a width, w, for the peak of the ionization rate curve as a function of distance, as the distance between points where I is a maximum and half of this value. The value of ionization zone width calculated for the case of Figure 2 was 0.40 $\mathring{A}$.

III. DISCUSSION AND CONCLUSION

The calculate of the ionization rate constants of hydrogenic atoms were realized previously by several authors. Haydock and Kingham [9, 10] developed a convenient JWKB method and tunneling potential that inspired several works [11]. In this formulation the tunneling rate constant is given by,

$$\begin{aligned} R \;=\; & A^2\nu \int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi/2} \sin\theta d\theta d\phi \times \\ & \times\ \exp\left(-2^{\frac{3}{2}}\int_{r_o(\theta,\phi)}^{r_1(\theta,\phi)}[V(r,\theta,\phi)-E]^{1/2}dr\right)\ . \end{aligned} \tag{16}$$

where $A^2\nu$ is a numerical prefactor, $V(r,\theta,\phi)$ is the potential energy, $r_o(\theta,\phi)$ and $r_1(\theta,\phi)$ are, respectively, the inner and outer classical turning points along the direction $(\theta,\ \phi)$.

Lam and Needs [12] using the JWKB method presented in reference [10] show that Haydock and Kingham expression for the tunneling rate constant in the FIM is inaccurate and derived one expression more accurate. In reference [13] is realized a numerical calculations for the ionization rate. In this work, the authors consider that the electric field varies along the potential barrier.

In this paper we present an analytical calculation of ionization rate constant which combines mathematical simplicity with reasonable accuracy.

Despite its simplicity, the model proposed in this work contains the important physical characteristics of the problem of field ionization near a metal surface. In general, the articles inspired by reference [10] take the factor $A^2\nu$ like 1. In our model, the final expressions there are no numerical factors to be determined.

In conclusion we have performed the field ionization rate-constants near a metal surface. A new analytic formula is given for the ionization rate-constant of an atom as a function from the metal surface and the width of the ionization zone is calculated.

The clarity of approach and mathematical ease of the method is shown to be compatible with the production of acceptably results.

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