Electric field and energy of a point electric charge between confocal hyperboloidal electrodes

E. Ley-Koo
Instituto de Física, Universidad Nacional Autónoma de México
Apartado Postal 20-364, 01000 México, D.F., Mexico

Recibido el 18 de enero de 2001; aceptado el 22 de enero de 2001

The electric potential and intensity fields, as well as the energy of a point electric charge between confocal hyperboloidal electrodes is evaluated as a superposition of prolate spheroidal harmonics using the Green-function technique. This study is motivated by the need to model the electric field between the tip and the sample in a scanning tunneling microscope, and it can also be applied to a conductor-insulator-conductor junction.

Keywords: Electric field and energy; scanning tunneling microscopy

Los campos de potencial y de intensidad eléctrica, así como la energía de una carga eléctrica puntual entre electrodos hiperboloidales confocales se evaluan como superposiciones de armónicos esferoidales prolatos usando la técnica de la función de Green. Este estudio ha sido motivado por la necesidad de modelar el campo eléctrico entre la punta y la muestra de un microscopio de tunelamiento y barrido, y se puede aplicar también a una unión de conductor-aislante-conductor.

Descriptores: Campo y energía eléctricos; microscopía de barrido y tunelamiento

PACS: 41.10.Dq

1. Introduction

The writing of this paper was motivated by the work "Tip-to-surface distance variations vs voltage in scanning tunneling microscopy (STM)" of Seine *et al.* [1]. The authors describe the STM junction geometry in terms of a tip shaped as a hyperboloid of revolution and of a sample surface as an infinite plane (that can be regarded as a particular case of a hyperboloid). The problem then consists in determining the electric potential between both electrodes. They consider such a potential to be the sum of electrostatic and image potentials. The electrostatic potential is given in Ref. 1 as an analytical expression citing [2], which is inconsistent in their use of the hyperboloidal coordinate and in their application to non-confocal hyperboloids as commented in Refs. 3 and 4. The authors of Ref. 1 also introduce a modified three-dimensional Simmons model for the image potential, recognizing that the original Simmons model deals with plane junctions [5, 6] and making the modifications for the hyperboloidal geometry. They also state "The exact form of the image potential for this geometry has not been computed".

The purpose of this paper is to show how the electric potential of a point charge between two confocal hyperboloidal electrodes, each at a fixed potential, can be constructed as a superposition of prolate spheroidal harmonics using the standard Green-function technique [7]. The construction is carried out by obtaining the general solutions of the Laplace equation and in particular the electrostatic potential arising from the potential difference between the electrodes, in Sec. 2. The Dirichlet Green function, or potential of a unit point charge between the grounded electrodes, is constructed as a series of prolate spheroidal harmonics in Sec. 3. The electric potential and intensity fields of an electron between the grounded electrodes, and the induced charges on the electrodes are evaluated in Sec. 4. The potential arising from the induced charges and the energy of interaction of the electron with such charges are evaluated in Sec. 5. The closing section contains a discussion of several points of didactic value and about the specific applications to STM and conductor-insulator-conductor junctions.

2. Separation and solutions of Laplace equation in prolate spheroidal coordinates

The prolate spheroidal coordinates (η, ξ, φ) are defined through the transformation equations to cartesian coordinates [8]

$$x = c\sqrt{(\eta^2-1)(1-\xi^2)}\ \cos\varphi,$$
$$y = c\sqrt{(\eta^2-1)(1-\xi^2)}\ \operatorname{sen}\varphi,$$
$$z = c\,\eta\,\xi. \qquad (1)$$

The constant parameter c determines the positions of the focii ($x = 0$, $y = 0$, $z = \pm c$) on the z-axis. Each value of $1 \leq \eta < \infty$ defines a prolate spheroidal surface centered at the origin with a major axis $2c\eta$ along the z-axis and minor axes $2c(\eta^2 - 1)^{1/2}$ in the x-y plane. Each value of $-1 \leq \xi \leq 1$ defines a hyperboloid of revolution with center at the origin, a real axis $2c\xi$ along the z-axis and imaginary axes $2c(1 - \xi^2)^{1/2}$ in the x-y plane; the x-y plane corresponds to $\xi = 0$, and the hyperboloids with $\xi > 0$ and $\xi < 0$ open upwards and downwards, respectively. The coordinate $0 \leq \varphi \leq 2\pi$ is the usual azimuthal angle, and each of its values defines a meridian half-plane. For example, $(1 \leq \eta < \infty, \xi \approx 1, 0 \leq \varphi \leq 2\pi)$ models the tip of the STM and $(1 \leq \eta < \infty, \xi = 0, 0 \leq \varphi \leq 2\pi)$ the plane surface of the sample.

The evaluation of the differential displacement

$$d\vec{r} = \hat{\imath}\, dx + \hat{\jmath}\, dy + \hat{k}\, dz = \hat{\eta}\, h_\eta\, d_\eta + \hat{\xi}\, h_\xi\, d_\xi + \hat{\varphi}\, h_\varphi\, d_\varphi \quad (2)$$

leads to the identification of the scale factors

$$h_\eta = c\sqrt{\frac{\eta^2-\xi^2}{\eta^2-1}}, \qquad h_\xi = c\sqrt{\frac{\eta^2-\xi^2}{1-\xi^2}}, \qquad h_\varphi = c\sqrt{(\eta^2-1)(1-\xi^2)} \quad (3)$$

and the orthogonal unit vectors

$$\hat{\eta} = \frac{\eta\sqrt{1-\xi^2}\,(\hat{\imath}\cos\varphi + \hat{\jmath}\,\mathrm{sen}\,\varphi) + \xi\sqrt{\eta^2-1}\,\hat{k}}{\sqrt{\eta^2-\xi^2}},$$

$$\hat{\xi} = \frac{-\xi\sqrt{\eta^2-1}\,(\hat{\imath}\cos\varphi + \hat{\jmath}\,\mathrm{sen}\,\varphi) + \eta\sqrt{1-\xi^2}\,\hat{k}}{\sqrt{\eta^2-\xi^2}},$$

$$\hat{\varphi} = -\hat{\imath}\,\mathrm{sen}\,\varphi + \hat{\jmath}\cos\varphi. \quad (4)$$

Correspondingly, the Laplace equation takes the explicit form

$$\left\{\frac{1}{c^2(\eta^2-\xi^2)}\left[\frac{\partial}{\partial\eta}(\eta^2-1)\frac{\partial}{\partial\eta} + \frac{\partial}{\partial\xi}(1-\xi^2)\frac{\partial}{\partial\xi}\right] + \frac{1}{c^2(\eta^2-1)(1-\xi^2)}\frac{\partial^2}{\partial\varphi^2}\right\} f(\eta,\xi,\varphi) = 0. \quad (5)$$

It admits separable solutions of the type

$$f(\eta,\xi,\varphi) = H(\eta)\Xi(\xi)\Phi(\varphi)$$

in which each factor satisfies the respective ordinary differential equation

$$\left[\frac{d}{d\eta}(\eta^2-1)\frac{d}{d\eta} - \frac{m^2}{\eta^2-1}\right]H(\eta) = \ell(\ell+1)H(\eta), \quad (6)$$

$$\left[\frac{d}{d\xi}(1-\xi^2)\frac{d}{d\xi} - \frac{m^2}{1-\xi^2}\right]\Xi(\xi) = -\ell(\ell+1)\Xi(\xi), \quad (7)$$

$$\frac{d^2\Phi}{d\varphi^2} = -m^2\Phi. \quad (8)$$

Both Eqs. (6) and (7) are identified as the Legendre equation in the respective intervals $1 \le \eta < \infty$ and $-1 \le \xi \le 1$, and Eq. (8) and its solutions are well-known. Therefore, the general solution of Eq. (5) can be written as

$$f(\eta,\xi,\varphi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\left[A_\ell^m P_\ell^m(\eta) + B_\ell^m(\eta)\right] \times \left[C_\ell^m P_\ell^m(\xi) + D_\ell^m Q_\ell^m(\xi)\right] e^{im\varphi} \quad (9)$$

in terms of the Legendre functions of the first and second kinds.

As an illustration, we can evaluate the electrostatic potential $\Phi_{\rm es}(\eta,\xi,\varphi)$ associated with the hyperboloidal electrodes $\xi=\xi_1$ and $\xi=\xi_2$ kept at the potentials V_1 and V_2, respectively. The boundary conditions

$$\phi_{\rm es}(\eta,\xi=\xi_1,\varphi) = V_1 \quad \text{and} \quad \phi_{\rm es}(\eta,\xi=\xi_2,\varphi) = V_2 \quad (10)$$

exclude the η and φ dependent terms in Eq. (9), thereby restricting the solutions to the lowest harmonic with $\ell = 0$ and $m = 0$, and in addition $B_o^o = 0$. Then the electrostatic potential satisfying Eqs. (10) takes the explicit form

$$\phi_{\rm es}(\eta,\xi,\varphi) = V_1\frac{Q_o(\xi_2)-Q_o(\xi)}{Q_o(\xi_2)-Q_o(\xi_1)} + V_2\frac{Q_o(\xi)-Q_o(\xi_1)}{Q_o(\xi_2)-Q_o(\xi_1)}. \quad (11)$$

In particular, the solution for the STM follows by taking $\xi_1 = 0$ for the sample surface and $\xi_2 \approx 1$ for the microscope tip. The reader has already been warned [3,4] about the inconsistent uses of the hyperboloidal coordinate and of the electrostatic potential for confocal hyperboloidal electrodes in Ref. 1.

3. Construction of the Dirichlet Green function for confocal hyperboloidal boundaries

The Green function satisfies the Poisson equation for a unit point charge [7]

$$\left\{\frac{1}{c^2(\eta^2-\xi^2)}\left[\frac{\partial}{\partial\eta}(\eta^2-1)\frac{\partial}{\partial\eta} + \frac{\partial}{\partial\xi}(1-\xi^2)\frac{\partial}{\partial\xi}\right] + \frac{1}{c^2(\eta^2-1)(1-\xi^2)}\frac{\partial^2}{\partial\varphi^2}\right\} G(\eta,\xi,\varphi;\eta',\xi',\varphi') = -4\pi\frac{\delta(\eta-\eta')\,\delta(\xi-\xi')\,\delta(\varphi-\varphi')}{h_\eta h_\xi h_\varphi}. \quad (12)$$

The Dirichlet Green function of interest in this work satisfies the boundary conditions of grounded confocal hyperboloidal electrodes

$$G_{\rm D}(\eta,\xi=\xi_1,\varphi;\eta',\xi',\varphi') = 0$$

and

$$G_{\rm D}(\eta,\xi=\xi_2,\varphi;\eta',\xi',\varphi') = 0. \quad (13)$$

Since Eq. (12) reduces to Eq. (5) for all points of space except the position of the point source (η',ξ',φ') its solutions are of the harmonic type of Eq. (9). The boundary conditions of Eqs. (13) can be satisfied by applying them to the ξ dependent functions

$$C_\ell^m P_\ell^m(\xi_1) + D_\ell^m Q_\ell^m(\xi_1) = 0$$

and

$$C_\ell^m P_\ell^m(\xi_2) + D_\ell^m Q_\ell^m(\xi_2) = 0. \quad (14)$$

This is a set of two algebraic linear homogeneous equations in the unknown coefficients C_ℓ^m and D_ℓ^m. It has nontrivial and nonvanishing solutions only if its determinant vanishes

$$P_\ell^m(\xi_1)Q_\ell^m(\xi_2) - Q_\ell^m(\xi_1)P_\ell^m(\xi_2) = 0. \quad (15)$$

This happens only for an infinite set of discrete values

$$\ell = \lambda_s, \quad s = 1, 2, 3, \ldots, \quad (16)$$

which are not necessarily integer numbers. These values have to be determined by solving numerically the trascendental Eq. (15) using the hypergeometric function representations of the Legendre functions [9]. The ratio of the unknown coefficients follows from Eqs. (14) and (15) and can be written in two equivalent forms

$$\frac{C_\ell^m}{D_\ell^m} = -\frac{Q_\ell^m(\xi_1)}{P_\ell^m(\xi_1)} = -\frac{Q_\ell^m(\xi_2)}{P_\ell^m(\xi_2)}. \quad (17)$$

Correspondingly, the ξ dependent functions can be written in the alternative forms

$$\begin{aligned}\Xi_{\lambda_s}^m(\xi) &= N_{\lambda_s}^m \left[Q_{\lambda_s}^m(\xi_2)P_{\lambda_s}^m(\xi) - P_{\lambda_s}^m(\xi_2)Q_{\lambda_s}^m(\xi)\right] \\ &= \bar{N}_{\lambda_s}^m \left[P_{\lambda_s}^m(\xi_1)\, Q_{\lambda_s}^m(\xi) - Q_{\lambda_s}^m(\xi_1)\, P_{\lambda_s}^m(\xi)\right], \quad (18)\end{aligned}$$

which are solutions of Eq. (7), satisfy obviously the boundary conditions of Eqs. (14), and are orthonormal in the interval $\xi_1 \le \xi \le \xi_2$

$$\int_{\xi_1}^{\xi_2} d\xi \Xi_{\lambda_s}^m(\xi)\Xi_{\lambda_{s'}}^m(\xi) = \delta_{ss'}. \quad (19)$$

The orthogonality follows from the identification of Eq. (7) as and eigenvalue problem and the normalization constants in Eqs. (18) can be choosen to ensure that the integral of Eq. (19) is one when $s = s'$

The orthonormal set of prolate spheroidal harmonic functions, which are the product of the ξ dependent functions of Eq. (18) and the orthonormal Fourier functions in the azimuthal angle, is also a complete set

$$\sum_{s=1}^{\infty}\sum_{m=-\infty}^{\infty} \Xi_{\lambda_s}^m(\xi')\Xi_{\lambda_s}^m(\xi)\frac{e^{im(\varphi-\varphi')}}{2\pi} = \delta(\xi-\xi')\,\delta(\varphi-\varphi'). \quad (20)$$

Then the solution of Eq. (12) can be written as a series of these prolate spheroidal harmonics, incorporating the symmetry of the Green function under the exchange of the field and source points

$$G_D(\eta,\xi,\varphi;\eta',\xi',\varphi') = \sum_{s=1}^{\infty}\sum_{m=-\infty}^{\infty} g_{\lambda_s}^m(\eta,\eta')\,\Xi_{\lambda_s}^m(\xi')\,\Xi_{\lambda_s}^m(\xi)\frac{e^{im(\varphi-\varphi')}}{2\pi}. \quad (21)$$

The "coefficients" in this series $g_{\lambda_s}^m(\eta,\eta')$ follow from the substitution of Eqs. (21), (20) and (3) in Eq. (12), using Eqs. (6)–(8) and the linear independence of the prolate spheroidal harmonics to obtain

$$\left[\frac{d}{d\eta}(\eta^2-1)\frac{d}{d\eta} - \lambda_s(\lambda_s+1) - \frac{m^2}{\eta^2-1}\right] g_{\lambda_s}^m(\eta,\eta') = -\frac{4\pi}{c}\delta(\eta-\eta'). \quad (22)$$

This equation for $\eta \neq \eta'$ reduces to Eq. (6), suggesting the choices

$$g_{\lambda_s}^m(\eta,\eta') = A_{\lambda_s}^m Q_{\lambda_s}^m(\eta')\,P_{\lambda_s}^m(\eta) \quad \text{for} \quad \eta \le \eta' \quad (23)$$

and

$$g_{\lambda_s}^m(\eta,\eta') = A_{\lambda_s}^m P_{\lambda_s}^m(\eta')\,Q_{\lambda_s}^m(\eta) \quad \text{for} \quad \eta \ge \eta', \quad (24)$$

which ensure the continuity of the Green function for $\eta = \eta'$ and its symmetry under the exchange of η and η'. The integration of Eq. (22) around $\eta = \eta'$

$$(\eta^2-1)\left.\frac{dg_{\lambda_s}^m(\eta,\eta')}{d\eta}\right|_{\eta=\eta'_+} - (\eta^2-1)\left.\frac{dg_{\lambda_s}^m(\eta,\eta')}{d\eta}\right|_{\eta=\eta'_-} = -\frac{4\pi}{c} \quad (25)$$

leads to the determination of the coefficient $A_{\lambda_s}^m$, using Eq. (24) for the first term and Eq. (23) for the second term

$$A_{\lambda_s}^m(\eta'^2-1)\left[P_{\lambda_s}^m(\eta')\frac{dQ_{\lambda_s}^m(\eta')}{d\eta'} - Q_{\lambda_s}^m(\eta')\frac{dP_{\lambda_s}^m(\eta')}{d\eta'}\right] = -\frac{4\pi}{c}. \quad (26)$$

The expression inside the brackets is the Wronskian for the Legendre functions which is equal to $-1/(\eta'^2-1)$, and therefore $A_{\lambda_s}^m$ is simply $4\pi/c$. Thus, the complete expression for the Dirichtet Green function is

$$G_D(\eta,\xi,\varphi;\eta',\xi',\varphi') = \frac{4\pi}{c}\sum_{s=1}^{\infty}\sum_{m=-\infty}^{\infty} P_{\lambda_s}^m(\eta_<)\,Q_{\lambda_s}^m(\eta_>)\,\Xi_{\lambda_s}^m(\xi')\,\Xi_{\lambda_s}^m(\xi)\frac{e^{im(\varphi-\varphi')}}{2\pi} \quad (27)$$

where $\eta_<$ and $\eta_>$ are the smaller and the larger of η and η'.

4. Electric potential field intensity and induced charges for an electron between grounded confocal hyperboloidal electrodes

When an electron is located between the grounded confocal hyperboloidal electrodes, the electric potential of the system is given by the product of the charge of the electron and the Dirichlet Green function constructed in the previous section

$$\phi(\eta,\xi,\varphi;\eta_e,\xi_e,\varphi_e) = -eG_D(\eta,\xi,\varphi;\eta_e,\xi_e,\varphi_e) = -\frac{4\pi e}{c}\sum_{s=1}^{\infty}\sum_{m=-\infty}^{\infty} P_{\lambda_s}^m(\eta_<)\, Q_{\lambda_s}^m(\eta_>)\, \Xi_{\lambda_s}^m(\xi_e)\, \Xi_{\lambda_s}^m(\xi)\frac{e^{im(\varphi-\varphi_e)}}{2\pi}. \quad (28)$$

This potential is the superposition of the Coulomb potential of the electron and the potential associated with the charges induced in the electrodes.

In scanning tunneling microscopy and conductor-insulator-conductor junctions the energy of interaction of the electron with the charges induced on the electrodes is one of the important contributions to the barrier to be tunneled through. The evaluation of this energy contribution could be attempted by evaluating the energy of the electron in the potential of Eq. (28) and substracting the energy of the electron in its own Coulomb field, but the reader will realize that both enrgies are infinite. As anticipated in the Introduction, the evaluation of the potential due to the induced charges and the energy of interaction of the electron with them will be presented in Sec. 5. Such an evaluation requires the previous determination of the electric field intensity and charge distributions on the electrodes, which is done in the remaining of this section.

The electric field intensity is obtained as the negative gradient of the potential of Eq. (28),

$$\begin{aligned}\vec{E}(\eta,\xi,\varphi;\eta_e,\xi_e,\varphi_e) &= -\left[\frac{\hat{\eta}}{h_\eta}\frac{\partial}{\partial\eta} + \frac{\hat{\xi}}{h_\xi}\frac{\partial}{\partial\xi} + \frac{\hat{\varphi}}{h_\varphi}\frac{\partial}{\partial\varphi}\right]\phi(\eta,\xi,\varphi;\eta_e,\xi_e,\varphi_e) \\ &= \frac{4\pi e}{c}\sum_{s=1}^{\infty}\sum_{m=-\infty}^{\infty}\left\{\frac{\hat{\eta}}{h_\eta}\frac{d}{d\eta}\left[P_{\lambda_s}^m(\eta_<)\, Q_{\lambda_s}^m(\eta_>)\right]\Xi_{\lambda_s}^m(\xi)\right. \\ &\quad \left. + \frac{\hat{\xi}}{h_\xi}P_{\lambda_s}^m(\eta_<)\, Q_{\lambda_s}^m(\eta_>)\frac{d\Xi_{\lambda_s}^m(\xi)}{d\xi} + \frac{\hat{\varphi}}{h_\varphi}P_{\lambda_s}^m(\eta_<)\, Q_{\lambda_s}^m(\eta_>)\, \Xi_{\lambda_s}^m(\xi)\, \mathrm{im}\right\}\Xi_{\lambda_s}^m(\xi_e)\frac{e^{im(\varphi-\varphi_e)}}{2\pi}. \quad (29)\end{aligned}$$

Two observations about this expression are pertinent at this moment. The components in $\hat{\eta}$ show a discontinuity at $\eta = \eta_e$ and lead upon integration over the area of any closed surface containing the point $(\eta = \eta_e, \xi = \xi_e, \varphi = \varphi_e)$ to $-4\pi e$, in agreement with Gauss' law. The components of the field in $\hat{\eta}$ and $\hat{\varphi}$ at the positions of the electrodes $\xi = \xi_1$ and $\xi = \xi_2$ vanish on account of Eq. (18), and its net components in $\hat{\xi}$ are perpendicular to the grounded hyperboloidal electrodes. The latter serve to evaluate the surface charge density distributions on the respective electrodes, by applying Gauss law

$$\sigma(\eta,\xi=\xi_1,\varphi) = \frac{\hat{\xi}\cdot\vec{E}(\eta,\xi=\xi_1,\varphi)}{4\pi} = \frac{e}{c}\sum_{s=1}^{\infty}\sum_{m=-\infty}^{\infty} P_{\lambda_s}^m(\eta_<)\, Q_{\lambda_s}^m(\eta_>)\, \Xi_{\lambda_s}^m(\xi_e)\left.\frac{d\Xi_{\lambda_s}^m(\xi)}{h_\xi d\xi}\right|_{\xi=\xi_1}\frac{e^{im(\varphi-\varphi_e)}}{2\pi}, \quad (30)$$

$$\sigma(\eta,\xi=\xi_2,\varphi) = -\frac{\hat{\xi}\cdot\vec{E}(\eta,\xi=\xi_2,\varphi)}{4\pi} = -\frac{e}{c}\sum_{s=1}^{\infty}\sum_{m=-\infty}^{\infty} P_{\lambda_s}^m(\eta_<)\, Q_{\lambda_s}^m(\eta_>)\, \Xi_{\lambda_s}^m(\xi_e)\left.\frac{d\Xi_{\lambda_s}^m(\xi)}{h_\xi d\xi}\right|_{\xi=\xi_2}\frac{e^{im(\varphi-\varphi_e)}}{2\pi}. \quad (31)$$

The total charges on each electrode are obtained by integrating Eqs. (30)–(31) over the respective surfaces

$$Q_i = \frac{e}{c}\sum_{s=1}^{\infty}\sum_{m=-\infty}^{\infty}\int_1^{\infty}\int_0^{2\pi} h_\eta d\eta h_\varphi d\varphi P_{\lambda_s}^m(\eta_<)\, Q_{\lambda_s}^m(\eta_>)\, \Xi_{\lambda_s}^m(\xi_e)\frac{1}{h_\xi}\left.\frac{d\Xi_{\lambda_s}^m}{d\xi}\right|_{\xi=\xi_i}\frac{e^{im(\varphi-\varphi_e)}}{2\pi} \quad (32)$$

for $i = 1, 2$. The combination of the scale factors using Eqs. (3) is

$$\frac{h_\xi h_\varphi}{h_\xi} = c\left(1-\xi_i^2\right). \quad (33)$$

On the other hand the derivatives of the ξ dependent functions evaluated from Eqs. (18) are the Wronskians of the Legendre functions

$$\frac{d\Xi_{\lambda_s}^m(\xi_1)}{d\xi_1} = \bar{N}_{\lambda_s}^m\left[P_{\lambda_s}^m(\xi_1)\frac{dQ_{\lambda_s}^m(\xi_1)}{d\xi_1} - Q_{\lambda_s}^m(\xi_1)\frac{dP_{\lambda_s}^m(\xi_1)}{d\xi_1}\right] = \bar{N}_{\lambda_s}^m(1-\xi_1^2)^{-1}$$

and

$$\frac{d\Xi_{\lambda_s}^m(\xi_2)}{d\xi_2} = N_{\lambda_s}^m\left[Q_{\lambda_s}^m(\xi_2)\frac{dP_{\lambda_s}^m(\xi_2)}{d\xi_2} - P_{\lambda_s}^m(\xi_2)\frac{dQ_{\lambda_s}^m(\xi_2)}{d\xi_2}\right] = -N_{\lambda_s}^m(1-\xi_2^2)^{-1}. \quad (34)$$

The integration over the azimuthal angle in Eq. (33) selects only the term with $m = 0$. The integration over the spheroidal coordinate η can be performed from Eq. (6) giving the reciprocal of the eigenvalue. Then the expressions for the charges on the electrodes become

$$Q_1 = e\sum_{s=1}^{\infty}\frac{\bar{N}_{\lambda_s}\Xi_{\lambda_s}(\xi_e)}{\lambda_s(\lambda_s+1)}, \quad Q_2 = e\sum\frac{N_{\lambda_s}\Xi_{\lambda_s}(\xi_e)}{\lambda_s(\lambda_s+1)}. \quad (35)$$

And the sum of the charges induced in the grounded electrodes is

$$Q_1 + Q_2 = e\sum_{s=1}^{\infty}\frac{(\bar{N}_{\lambda_s}+N_{\lambda_s})\,\Xi_{\lambda_s}(\xi_e)}{\lambda_s(\lambda_s+1)}. \quad (36)$$

It is straightforward to check that the sum in Eq. (36) is the representation of 1 as a series in the basis of orthonormal functions of Eq. (18), for any position of the electron $\xi = \xi_e$, so that the total induced charge is e.

5. Electric potential due to induced charges and energy of interaction with the electron

The surface charge densities induced by the electron in the electrodes, Eqs. (30)–(31), and the free space Green function expressed as a prolate spheroidal harmonic series

$$G_F(\eta,\xi,\varphi;\eta',\xi',\varphi') \equiv \frac{1}{|\vec{r}-\vec{r}'|} = \frac{4\pi}{c}\sum_{\ell=0}^{\infty}\sum_{\mu=-\ell}^{\ell} P_\ell^\mu(\eta_<)\,Q_\ell^\mu(\eta_>)\,N_\ell^\mu P_\ell^\mu(\xi')\,N_\ell^\mu P_\ell^\mu(\xi)\frac{e^{i\mu(\varphi-\varphi')}}{2\pi} \quad (37)$$

are the ingredients to evaluate the electric potential of those charges

$$\phi_{\text{ind}}(\eta,\xi,\varphi) = \sum_{i=1}^{2}\int_1^\infty\int_0^{2\pi} h_{\eta'}\,d\eta'\,h_{\varphi'}\,d\varphi'\,G_F(\eta,\xi,\varphi;\eta',\xi',\varphi')\,\sigma(\eta',\xi',\varphi')\Big|_{\xi'=\xi_i} \quad (38)$$

by integrating their product over the areas of both electrodes. Notice that the combination of the scale factors in Eq. (38), including the one in Eqs. (30)–(31), is the same one as that of Eq. (33); and also the derivatives of Eqs. (34) are common to the integrals of Eqs. (32) and (38). The integration over the azimuthal angle φ' leads to the selection rule $\mu = m$ for the sums from Eqs. (37) and (30). The integration over the spheroidal coordinate η' requires distinguishing the cases of $\eta \le \eta_e$ and $\eta \ge \eta_e$, and dividing the interval $1 \le \eta' < \infty$ in three subintervals for each case. The integrals of the products of two Legendre functions one of order ℓ and the other of order λ_s have closed forms obtainable from the respective differential equations of the type of Eq. (6). The final result is

$$\phi_{\text{ind}}(\eta \le \eta_e,\xi,\varphi) = \frac{4\pi e}{c}\sum_{\ell=0}^{\infty}\sum_{s=1}^{\infty}\sum_{m=-\ell}^{\ell}\left[\bar{N}_{\lambda_s}^m N_\ell^m P_\ell(\xi_1) + N_{\lambda_s}^m N_\ell^m P_\ell^m(\xi_2)\right] \times \Xi_{\lambda_s}^m(\xi_e)\frac{Q_\ell^m(\eta_e)\,P_\ell^m(\eta) - Q_{\lambda_s}^m(\eta_e)\,P_{\lambda_s}^m(\eta)}{\lambda_s(\lambda_s+1)-\ell(\ell+1)}N_\ell^m P_\ell^m(\xi)\frac{e^{im(\varphi-\varphi_e)}}{2\pi}, \quad (39)$$

$$\phi_{\text{ind}}(\eta \ge \eta_e,\xi,\varphi) = \frac{4\pi e}{c}\sum_{\ell=0}^{\infty}\sum_{s=1}^{\infty}\sum_{m=-\ell}^{\ell}\left[\bar{N}_{\lambda_s}^m N_\ell^m P_\ell^m(\xi_1) + N_{\lambda_s}^m N_\ell^m P_\ell^m(\xi_2)\right] \times \Xi_{\lambda_s}^m(\xi_e)\frac{P_\ell^m(\eta_e)\,Q_\ell^m(\eta) - P_{\lambda_s}^m(\eta_e)\,Q_{\lambda_s}^m(\eta)}{\lambda_s(\lambda_s+1)-\ell(\ell+1)}N_\ell^m P_\ell^m(\xi)\frac{e^{im(\varphi-\varphi_e)}}{2\pi}. \quad (40)$$

The reader can check that this electric potentials is continuous at $\eta = \eta_e$. Also, the electric intensity field evaluated as the negative gradient of Eqs. (39)–(40) is continuous at the position of the electron $\vec{r}_e$. In this way, the electric potential of Eqs. (39)–(40) is equivalent to the difference between that of Eq. (28) and the electron Coulomb potential.

The energy of interaction of the electron and the charges induced in the electrodes is half the product of the charge of the electron and the electric potential of Eqs.(39)–(40) at the positon $\vec{r} = \vec{r}_e$

$$U_{\text{ind}}(\vec{r}_e) = -\frac{1}{2}e\phi_{\text{ind}}(\eta=\eta_e,\xi=\xi_e,\varphi=\varphi_e) = -\frac{e^2}{c}\sum_{\ell=0}^{\infty}\sum_{s=1}^{\infty}\sum_{m=-\ell}^{\ell}\left[\bar{N}_{\lambda_s}^m N_\ell^m P_\ell^m(\xi_1) + N_{\lambda_s}^m N_\ell^m P_\ell^m(\xi_2)\right] \times\Xi_{\lambda_s}^m(\xi_e)\frac{P_\ell^m(\eta_e)\,Q_\ell^m(\eta_e) - P_{\lambda_s}^m(\eta_e)\,Q_{\lambda_s}^m(\eta_e)}{\lambda_s(\lambda_s+1)-\ell(\ell+1)}N_\ell^m P_\ell^m(\xi_e). \quad (41)$$

6. Discussion

Equations (11) and (39) describe the electrostatic potential due to the potential difference between the confocal hyperboloidal electrodes, and the electric potential due to the charges induced in the grounded electrodes by the presence of the electron between them, respectively. For the electron between the electrodes with a potential difference, the total electric potential is the superpositon of the electrostatic potential given by Eq. (11) and the electric potential of the electron between the grounded electrodes given by Eq. (28). The energy of the electron in such a situation is the sum of its electrostatic energy $-e\phi_{es}(\eta_e, \xi_e, \varphi_e)$ and its energy of interaction with the charges it induces in the electrodes of Eq. (41). These are the energy contributions to the potential barrier of interest in tunneling devices, such as STM and conductor-insulator-conductor junctions, modeled with confocal hyperboloidal electrodes. The detailed construction of the needed quantities to evaluate both energies has been carried out in Sec. 2 and 3 of this work, filling in the gap that was recognized in Ref. 1.

Some remarks are pertinent about the work of the *Centre d'Elaboration des Materiaux et d'Etudes Structurales* [1]. The electrostatic potential they use corresponds to Eq. (11), but with the wrong argument in the Legendre functions $Q_o(\cosh \xi)$. Their application of the same formula to nonconfocal hyperboloids does not satisfy the Laplace equation and is thereby not valid. Their extension of Simmons model for the image potential of plane junctions to the hyperboloidal geometry is based on the same assumption of nonconfocal hyperboloidal equipotentials, which can not be justified.

Some warnings about the terminology are also necessary. The term image potential was introduced by Simmons for parallel plane electrodes [5, 6]. For this geometry the method of images is applicable and the adjective is justified. However, Eqs. (6)–(8) [6] giving the explicit form of the image potential

$$V_i = \left(- \frac{e^2}{8\pi K \varepsilon_o} \right) \left\{ \frac{1}{2x} + \sum_{n=1}^{\infty} \left[\frac{ns}{(ns)^2 - x^2} - \frac{1}{ns} \right] \right\}$$

is not an electric potential. It is actually the energy of interaction of the electron with the image charges that it induces in the grounded plane electrodes. Since the method of images is not applicable to the hyperboloidal geometry, the use of the adjective image can be misleading. It is preferable to spell out the physical situation at hand to make it understandable, for instance Eq. (28) describes the electric potential of the electron between the grounded electrodes, Eqs. (38)–(40) describe the electric potential due to the charges induced in the electrodes, and Eq. (41) describes the energy of interaction of the electron and the induced charges.

In this work cgs electrostatic units have been used and the space between the electrodes is assumed to be empty. If such a space is filled in with a material with a dielectric constant K, the right hand sides of Eqs. (28) and (39)–(41) have to be divided by K.

The final remark is that Eqs. (11) and (41) are the correct and consistent descriptions of the electrostatic and induced charge energy contributions to the potential barrier for confocal hyperboloidal electrodes, which may serve as the starting point to redo the work of Ref. 1 and to analyze the tunneling in conductor-insulator-conductor junctions.

1. G. Seine *et al.*, *Phys. Rev. B* **60** (1999) 11045.
2. E. Durand, *Electrostatique*, (Masson, Paris, 1966), Vol. 2, p. 181.
3. E. Ley-Koo, "Modelación del campo eléctrico en microscopía de tunelamiento y barrido", *Memorias de la celebración de los Primeros Sesenta Años del Profesor Eliezer Braun*, (2000) en prensa.
4. E. Ley-Koo, Comment on "Tip-to-surface distance variations *vs*. voltage in scanning tunneling microscopy", *Phys. Rev. B* (in press).
5. J.G. Simmons, *J. Appl. Phys.* **34** (1963) 1793.
6. J.G. Simmons, *J. Appl. Phys.* **35** (1964) 2472.
7. J.D. Jackson, *Classical Electrodynamics*, Second Edition, (Wiley, New York, 1975).
8. G. Arfken, *Mathematical Methods for Physicists*, Second Edition, (Academic Press, New York, 1970), Chap. 2.
9. M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions*, (Dover, New York, 1965), Chap. 8.