

Methods for calculating electrostatic quantities due to a free charge in a nanoscale three-dimensional tip/base junction

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The exact solutions for fully three-dimensional electrostatic quantities due to a free charge in a nanoscale tip/base junction, such as the scanning-tunneling microscope, are given for the problem as modeled in the prolate-spheroidal coordinate system. These exact solutions consist of summation series of integrals of conical functions, and methods for calculating these exact solutions with high accuracy are described in detail in this paper. Calculated results for the surface-charge distribution on the tip and the base due to a free electron in a nanoscale tip/base junction are also presented. This analysis has important implications for the ultimate objective of quantifying electron tunneling, from first principles, in nonplanar geometries such as sharp vacuum field emitters. © 1995 American Institute of Physics.

I. INTRODUCTION

Fully three-dimensional nanoscale microelectronic structures have significant and practical applicability in the areas of very high-speed switching devices, intense electron/ion sources, and advanced image-display devices (e.g., HDTV), among other applications.^{1,2} Consequently, it is desirable to develop the capability to calculate the tunneling current of three-dimensional nanoscale electronic structures from first principles. However, devices such as these, utilizing atomically sharp field-emission tips, are inherently nonplanar geometries and they exhibit tunnel currents which are substantially larger than predicted by planar or one-dimensional models.³

An important first step in extending the analysis of electron tunneling beyond the often-used one-dimensional analysis of the Fowler–Nordheim field-emission theory⁴ is the recent result reported by Pan *et al.* (1994)⁵ for an exact expression, in the prolate-spheroidal coordinate system, of the fully three-dimensional potential-energy barrier associated with emitter tips. The consequent detailed understanding of the three-dimensional electrostatic potential and related quantities is an essential theoretical element for the ultimate objective of quantifying axial (symmetric) and off-axis tunnel currents.

The exact solution for several quantities related to the electrostatic interaction of a free electron in a biased tip/base junction, modeled in the prolate-spheroidal coordinate system, has been derived by two independent methods.^{5,6} The three-dimensional electrostatic potential V due to a free charge in a tip/base junction was derived using a classical separation-of-variables approach in Pan *et al.*⁵ where computed results for this quantity are given. The Green's function for the region between the tip and the base, modeled in the prolate-spheroidal coordinate system, is derived in Peridier *et al.*;⁶ this result might enable one, for example, to

model electron tunneling in a region with a charge *distribution* such as that which would occur in the situation of tunneling through physical medium as opposed to vacuum. This second paper⁶ also includes calculations for the potential-energy barrier Φ at on-axis and several off-axis sites in the tip/base geometry. Both analyses account properly for the effects of the image and multiple-image interactions that would occur in the limiting cases when the tip/anode spacing is $O(100 \text{ \AA})$, such as in the situation of scanning tunneling microscopy (STM).

The derived expressions for every electrostatic quantity in both papers^{5,6} include a summation series of integrals of conical functions K_r^m , and while computed results were given in each paper the numerical methods were not described. The intention of *this* paper is to describe the specific numerical methods required to accurately calculate the electrostatic quantities derived in Refs. 5 and 6. In addition, computed results for the surface-charge distributions, induced on both the tip and base surfaces by a free electron in the tip/base junction, are presented here.

II. PRIOR STUDIES

He *et al.*⁷ recognized that the potential-energy barrier for electron tunneling in a tip/base junction might vary considerably from a potential-energy barrier determined from planar assumptions. He *et al.*⁷ obtained analytic expressions for the induced image potential due to a free charge on the axis of symmetry of an STM tip in free space, modeled variously as a cone, hyperboloid, paraboloid, and as a sphere on the tip of a cone. However, it is worthwhile to note that this aforementioned analysis⁷ is fundamentally a one-dimensional study because only free-charge locations on the symmetry axis of the tip/base junction were considered. Furthermore, the result of He *et al.*⁷ is somewhat difficult to interpret given that the induced surface charge was considered on the tip surface only of the tip/base junction, but not on the base. (Physically, of course, the surface-charge distributions on the

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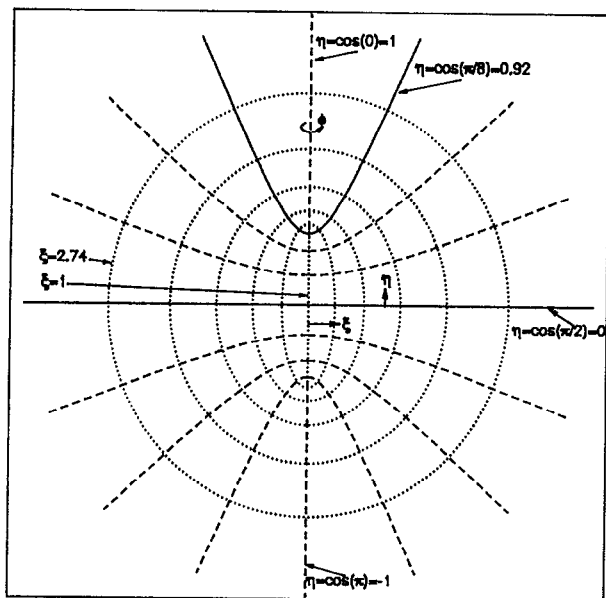


FIG. 1. The prolate-spheroidal coordinate system. Hyperboloid surfaces appropriate for modeling a tip/base junction are shown in dark print.

tip and the base are influenced both by: (i) the free electron in the junction, and (ii) by the surface-charge distribution on the opposing surface.)

III. THE THREE-DIMENSIONAL PROLATE-SPHEROIDAL MODEL OF A TIP/BASE JUNCTION

In our model the junction of the tip and the base is modeled as a region bounded by two hyperboloids in the prolate-spheroidal coordinate system, which is given by (Ref. 8, p. 103–104)

$$\begin{aligned}x &= a \sinh(u) \sin(v) \cos(\phi), \\y &= a \sinh(u) \sin(v) \sin(\phi), \\z &= a \cosh(u) \cos(v).\end{aligned}\quad (1)$$

In this coordinate system a is one-half the distance between the foci for each hyperboloid surface; curves corresponding to constant v are hyperboloid surfaces, curves corresponding to constant u are prolate-spheroidal surfaces (see Fig. 1). The variable transformation

$$\begin{aligned}\xi &= \cosh(u), \\\eta &= \cos(v),\end{aligned}\quad (2)$$

generate a coordinate system given by

$$\begin{aligned}x &= a \sqrt{\xi^2 - 1} \sqrt{1 - \eta^2} \cos(\phi), \\y &= a \sqrt{\xi^2 - 1} \sqrt{1 - \eta^2} \sin(\phi), \\z &= a \xi \eta,\end{aligned}\quad (3)$$

with the corresponding coordinate metrics:

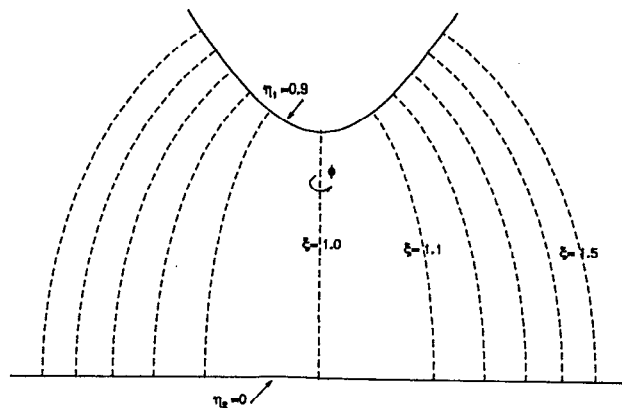


FIG. 2. The geometry for the model problem.

$$\begin{aligned}h_\xi &= a \sqrt{(\xi^2 - \eta^2)/(\xi^2 - 1)}, \\h_\eta &= a \sqrt{(\xi^2 - \eta^2)/(1 - \eta^2)}, \\h_\phi &= a \sqrt{(\xi^2 - 1)(1 - \eta^2)}.\end{aligned}\quad (4)$$

To model a tip/base junction in this prolate-spheroidal coordinate system two level hyperboloid surfaces of η are taken, one to represent the tip (say, at $\eta_1 = 0.9$) and the second to represent the base. (A flat anode would be represented by $\eta_2 = 0$.) In the new coordinate system, the range of the variables which define the junction or region between these two hyperboloid surfaces is

$$\begin{aligned}\phi &\in [0, 2\pi], \\\xi &\in [1, \infty), \\\eta &\in [\eta_1, \eta_2].\end{aligned}\quad (5)$$

This tip/base model in the prolate-spheroidal geometry is shown in Fig. 2, with lines of constant ξ given for $\xi = \{1.0(0.1)1.5\}$. It is worthwhile to note that the radius of curvature r_1 of the tip modeled in this fashion is

$$r_1 = a \sin(\theta_1) \tan(\theta_1), \quad (6)$$

while the cone angle of the tip θ_1 (defined as one-half of the angle subtended by the asymptotes of the hyperboloid surface) may be determined from

$$\theta_1 = \cos^{-1}(\eta_1). \quad (7)$$

Furthermore, in this model the separation distance d_{sep} of the tip from the flat surface is

$$d_{\text{sep}} = a \eta_1. \quad (8)$$

Consequently, it is worthwhile to note that in this prolate-spheroidal model only two among the three geometric parameters radius of curvature (r_1), tip cone angle (θ_1), and separation distance (d_{sep}), are independent, because fixing two of these three parameters automatically determines the third.

If a charge of strength q is placed at an arbitrary location $\mathbf{x}_c$ in a voltage-biased tip/base junction, the solution for the electrostatic potential V may be written as the sum of two subsidiary potentials

$$V = V_B + V_C, \quad (9)$$

where V_B is the potential due to the bias voltage V_0 applied across the junction, and V_C incorporates the effects of the free charge's interaction with the surface charges on the tip and base surfaces. The solutions for V_B, V_C are derived in Pan *et al.*⁵ and are

$$V_B = V_0 \frac{\ln\{[(1+\eta_2)/(1-\eta_2)][(1-\eta)/(1+\eta)]\}}{\ln\{[(1+\eta_2)/(1-\eta_2)][(1-\eta_1)/(1+\eta_1)]\}}, \quad (10)$$

$$V_C = \frac{q}{4\pi\epsilon_0|\mathbf{x}-\mathbf{x}_c|} + V_I, \quad (11)$$

with V_I being the interaction potential given by

$$V_I = \sum_{m=0}^{\infty} (2 - \delta_{0,m}) \cos(m\phi) \times \int_0^{\infty} [B_{\tau}^m K_{\tau}^m(\eta) + C_{\tau}^m K_{\tau}^m(-\eta)] K_{\tau}^m(\xi) d\tau. \quad (12)$$

In Eq. (12) the coefficients B_{τ}^m, C_{τ}^m are given by

$$B_{\tau}^m = \frac{q}{4\epsilon_0 a} \alpha_{\tau}^m [K_{\tau}^m(\xi_c) K_{\tau}^m(-\eta_2)] \times \left(\frac{K_{\tau}^m(\eta_c) K_{\tau}^m(-\eta_1) - K_{\tau}^m(-\eta_c) K_{\tau}^m(\eta_1)}{K_{\tau}^m(\eta_1) K_{\tau}^m(-\eta_2) - K_{\tau}^m(-\eta_1) K_{\tau}^m(\eta_2)} \right), \quad (13)$$

$$C_{\tau}^m = \frac{q}{4\epsilon_0 a} \alpha_{\tau}^m [K_{\tau}^m(\xi_c) K_{\tau}^m(\eta_1)] \times \left(\frac{K_{\tau}^m(-\eta_c) K_{\tau}^m(\eta_2) - K_{\tau}^m(\eta_c) K_{\tau}^m(-\eta_2)}{K_{\tau}^m(\eta_1) K_{\tau}^m(-\eta_2) - K_{\tau}^m(-\eta_1) K_{\tau}^m(\eta_2)} \right). \quad (14)$$

For expressions associated with V_C , the charge is located (without loss of generality) at $\mathbf{x}_c = (\xi_c, \eta_c, 0)$, and the coefficient term α_{τ}^m in expressions (13) and (14) is:

$$\alpha_{\tau}^m = \tau \frac{\tanh(\pi\tau)}{\cosh(\pi\tau)} \left[\frac{\Gamma(\frac{1}{2} + i\tau - m)}{\Gamma(\frac{1}{2} + i\tau + m)} \right]^2. \quad (15)$$

Here, Γ is the gamma function, and the method for calculating this quantity is given in Appendix A.

The expression K_{τ}^m in expressions (12), (13), and (14) is the "conical function" defined by

$$K_{\tau}^m(\mu) \equiv P_{-\frac{1}{2} + i\tau}^m(\mu); \quad (16)$$

conical functions are a special case of generalized Legendre functions which have an integer order m and a continuum of complex degrees of the form $(-\frac{1}{2} + i\tau)$, for $\tau \in [0, \infty)$. The second solution for $K_{\tau}^m(\mu)$ is $K_{\tau}^m(-\mu)$. Conical functions arise in the solution of the Laplace equation in the prolate-spheroidal coordinate system, and the numerical evaluation of these functions is described in Appendix B.

The potential-energy barrier Φ for a charge tunneling from the tip to the base, located at $\mathbf{x}_c$ is derived in Pan *et al.*⁵ and is given by

$$\Phi = q(V_B + V_I). \quad (17)$$

Finally, the induced surface-charge distributions σ_1 on the tip, and σ_2 on the base, may be determined from

$$\sigma_j = -\epsilon_0 \frac{1}{h_{\eta}} \frac{\partial V}{\partial \eta} \bigg|_{\eta_j}, \quad (18)$$

where the metric h_{η} is given in Eq. (4). Taking the derivative of Eq. (9) with respect to η , evaluating the result at the tip η , and using the Wronskian identity¹⁰

$$W[K_{\tau}^m(\mu), K_{\tau}^m(-\mu)] = \frac{(-1)^m}{(1-\mu^2)} \frac{2 \cosh(\pi\tau)}{\pi} \frac{\Gamma(\frac{1}{2} + i\tau + m)}{\Gamma(\frac{1}{2} + i\tau - m)} \quad (19)$$

gives σ_1 , the tip surface-charge distribution:

$$\sigma_1 = \frac{-2\epsilon_0 V_0}{a} \frac{1}{\sqrt{\xi^2 - \eta_1^2} \sqrt{1 - \eta_1^2}} \frac{1}{\ln[(1+\eta_2)/(1-\eta_2)(1-\eta_1)/(1+\eta_1)]} + \frac{q}{2\pi a^2} \frac{1}{\sqrt{\xi^2 - \eta_1^2} \sqrt{1 - \eta_1^2}} \cdot \sum_{m=0}^{\infty} (-1)^m (2 - \delta_{0,m}) \times \cos(m\phi) \int_0^{\infty} d\tau \left\{ \tau \tanh(\pi\tau) \frac{\Gamma(\frac{1}{2} + i\tau - m)}{\Gamma(\frac{1}{2} + i\tau + m)} [K_{\tau}^m(\xi_c) K_{\tau}^m(\xi)] \left(\frac{K_{\tau}^m(-\eta_c) K_{\tau}^m(\eta_2) - K_{\tau}^m(\eta_c) K_{\tau}^m(-\eta_2)}{K_{\tau}^m(\eta_1) K_{\tau}^m(-\eta_2) - K_{\tau}^m(-\eta_1) K_{\tau}^m(\eta_2)} \right) \right\}. \quad (20)$$

Similarly, the surface-charge distribution σ_2 on the anode surface at η_2 is

$$\sigma_2 = \frac{-2\epsilon_0 V_0}{a} \frac{1}{\sqrt{\xi^2 - \eta_2^2} \sqrt{1 - \eta_2^2}} \frac{1}{\ln[(1+\eta_2)/(1-\eta_2)(1-\eta_1)/(1+\eta_1)]} + \frac{q}{2\pi a^2} \frac{1}{\sqrt{\xi^2 - \eta_2^2} \sqrt{1 - \eta_2^2}} \cdot \sum_{m=0}^{\infty} (-1)^m (2 - \delta_{0,m}) \times \cos(m\phi) \int_0^{\infty} d\tau \left\{ \tau \tanh(\pi\tau) \frac{\Gamma(\frac{1}{2} + i\tau - m)}{\Gamma(\frac{1}{2} + i\tau + m)} [K_{\tau}^m(\xi_c) K_{\tau}^m(\xi)] \left(\frac{K_{\tau}^m(-\eta_c) K_{\tau}^m(\eta_1) - K_{\tau}^m(\eta_c) K_{\tau}^m(-\eta_1)}{K_{\tau}^m(\eta_1) K_{\tau}^m(-\eta_2) - K_{\tau}^m(-\eta_1) K_{\tau}^m(\eta_2)} \right) \right\}. \quad (21)$$

In expressions (20) and (21) it is evident that the charge distributions on each surface depend on the applied bias-voltage V_0 , and on the free charge in the junction at $\mathbf{x}_c = (\xi_c, \eta_c, 0)$, and on the opposing surface.

The above expressions for the electrostatic field V [Eq. (9)], the electron-tunneling potential barrier Φ [Eq. (17)], and the surface-charge distributions on the tip and the base σ_1, σ_2 [Eqs. (20) and (21)] are exact. Computed results for V are given in Pan *et al.*,⁵ and computed results for Φ are given in Peridier *et al.*⁶ where the more generalized Green's-function result is described. Methods for calculating these quantities, as well as computed results for the surface-charge distributions σ_1, σ_2 induced by a free electron in the tip/base junction, are described below.

IV. NUMERICAL METHOD FOR CALCULATING ELECTROSTATIC QUANTITIES IN THE PROLATE-SPHEROIDAL COORDINATE SYSTEM

The expressions above for the electrostatic potential V [Eq. (9)], for the tunneling potential-energy barrier Φ [Eq. (17)], and for the induced surface-charge distributions σ_1, σ_2 [Eqs. (20) and (21)] are exact, and can in principle be calcu-

lated to arbitrary accuracy. However, each expression includes a term, similar in form for each expression, that is a summation series (over $m=0,1,2,\dots$) of integrals (taken over $\tau \in [0, \infty)$) of gamma functions Γ of complex arguments multiplied by conical functions K_τ^m . As a practical matter, the numerical evaluation of this term is not trivial and thus will be described in this section, using the expression V_I [Eq. (12)] as an example.

First, experience has demonstrated that, for evaluating an expression such as V_I [Eq. (12)], the result will converge faster if the summation operator is interchanged with the integral, i.e.,

$$V_{I,\text{calc}} = \frac{q}{4\epsilon_0 a} \int_0^\infty d\tau F(\tau), \quad (22)$$

with the argument of Eq. (22) given by the summation series

$$F(\tau) \equiv \sum_{m=0}^N s_m(\tau), \quad (23)$$

and each term $s_m(\tau)$ in the summation series $F(\tau)$ given by [see Eqs. (12), (13), (14), and (15)]

$$s_m(\tau) = (2 - \delta_{0,m}) \cos(m\phi) \tau \frac{\tanh(\pi\tau)}{\cosh(\pi\tau)} \left(\frac{\Gamma(\frac{1}{2} + i\tau - m)}{\Gamma(\frac{1}{2} + i\tau + m)} \right)^2 \frac{K_\tau^m(\xi_c) K_\tau^m(\xi)}{K_\tau^m(\eta_1) K_\tau^m(-\eta_2) - K_\tau^m(-\eta_1) K_\tau^m(\eta_2)} \{ [K_\tau^m(\eta) K_\tau^m(-\eta_2)] \\ \times [K_\tau^m(\eta_c) K_\tau^m(-\eta_1) - K_\tau^m(-\eta_c) K_\tau^m(\eta_1)] + [K_\tau^m(-\eta) K_\tau^m(\eta_1)] [K_\tau^m(-\eta_c) K_\tau^m(\eta_2) - K_\tau^m(\eta_c) K_\tau^m(-\eta_2)] \}. \quad (24)$$

The above expression for $V_{I,\text{calc}} \rightarrow V_I$ in the limit $N \rightarrow \infty$, where N is the number of terms taken in Eq. (23). Note that the field point is $\mathbf{x} = (\xi, \eta, \phi)$ and the location of the free charge is $\mathbf{x}_c = (\xi_c, \eta_c, 0)$ and that both are fixed constants; the dummy variable of integration is τ .

To calculate V_I from Eq. (22), $V_{I,\text{calc}}$, $F(\tau)$ was integrated using Simpson's Rule in steps of

$$\Delta\tau = 0.05; \quad (25)$$

the integration was carried out over successive intervals in $\tau \in [0,1]$, $\tau \in [1,2]$, $\tau \in [2,3]$, ..., until the magnitude of the last interval calculated was less than 10^{-9} of the magnitude of the total integrated result for $V_{I,\text{calc}}$. In practice the integration was typically terminated for $\tau \sim O(100)$. To calculate $F(\tau)$ at a specific value of τ the summation series given by expression (23) was summed for $N \leq 30$ terms; the mechanism for selecting N is described below. Each term $s_m(\tau)$ of expression (23) is the product of gamma functions Γ and conical function K_τ^m ; the method used to calculate the gamma function Γ is described in Appendix A, and procedures for calculating the conical function K_τ^m is discussed in Appendix B.

The number of terms N taken in the series to compute the integral-argument $F(\tau)$, defined by Eq. (23), was determined as follows. The summation terms $s_m(\tau)$ were calcu-

lated for $m=0,1,2,\dots,30$ and then, in the numerical procedure, each term $s_m(\tau)$ was compared to the $s_{m-1}(\tau)$ and $s_{m+1}(\tau)$ terms. The numerical behavior of these terms, illustrated schematically in Fig. 3, was as follows. For small or-

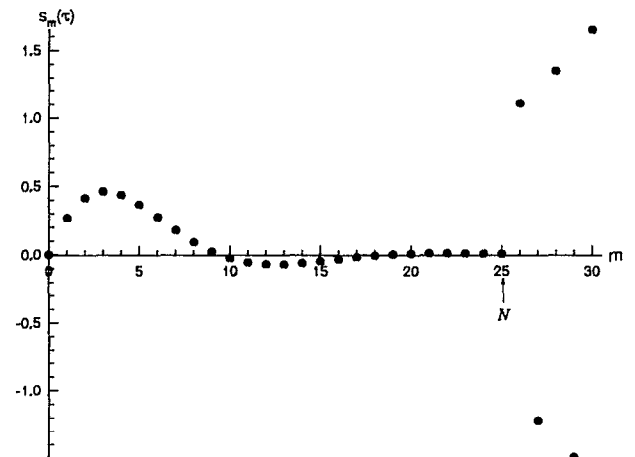


FIG. 3. Schematic showing the numerical character of subsequent terms $s_m(\tau)$ for increasing order m . In the schematic example illustrated here, the series solution for $F(\tau)$, Eq. (22), would be taken to $N=25$ terms.

der m the value of each term $s_m(\tau)$ was finite, with the magnitude of this term ultimately falling off for larger orders of m . However, for some values of $\mathbf{x}$ and $\mathbf{x}_c$, (particularly for $\mathbf{x}$ very close to $\mathbf{x}_c$, or $\mathbf{x}_c$ very close to a surface) after some term N subsequent terms of $s_m(\tau)$ alternated in sign and grew exponentially in magnitude. Consequently, each time $F(\tau)$ was calculated n was chosen to be the largest value of m prior to the onset of the exponential growth (or to 30 if no such growth occurred). Note that taking $m > 30$ results in a floating-point-overflow error when calculating the gamma function so it was convenient to terminate the series for a choice of $N \leq 30$. This numerical approach guarantees three to five significant digits of accuracy which is satisfactory for our purposes.

The method for calculating the electrostatic quantities that is described above and in Appendices A and B is estimated to yield three to five significant digits, with accuracy increasing as the distance of the field-point $\mathbf{x}$ from either the charge-location $\mathbf{x}_c$ or the boundary surfaces is increased. This estimate was obtained by numerical study of an exact expression given in van Nostrand¹⁰ for $1/|\mathbf{r}|$ as an expansion of integrals over associated conical functions:

$$\frac{1}{|\mathbf{x} - \mathbf{x}_c|} = \frac{\pi}{a} \sum_{m=0}^{\infty} (2 - \delta_{0,m}) \cos(m\phi) \times \int_0^{\infty} d\tau \alpha_{\tau}^m K_{\tau}^m(\xi) K_{\tau}^m(\xi_c) \times \begin{cases} K_{\tau}^m(\eta) K_{\tau}^m(-\eta_c) & \eta_c < \eta \\ K_{\tau}^m(-\eta) K_{\tau}^m(\eta_c) & \eta_c > \eta \end{cases} \quad (26)$$

The form of this expression is quite similar to that of the electrostatic quantities described above and, given the fact that $1/|\mathbf{r}|$ can be evaluated exactly, it was possible to directly evaluate the accuracy of the numerical-integration scheme by calculating expression (26) using the method described above and comparing the result to the exact solution.

V. CALCULATED RESULTS FOR THE SURFACE-CHARGE DISTRIBUTIONS σ_1, σ_2

Equation (20) was used to calculate the surface-charge distribution on the surface of the tip σ_1 , and Eq. (21) for the charge distribution σ_2 on the surface of the anode. Figure 4 illustrates both distributions for the case of zero applied voltage V_0 and thus the two surface-charge distributions are induced solely by the free electron. The tip in Fig. 4 is modeled as a level hyperboloid surface $\eta_1 = 0.9$ (which corresponds to a tip half angle of about 26°) and the charge is located at a point $\mathbf{x}_c = (\xi_c, \eta_c, \phi_c) = (13, .5, 0)$ in the tip/base junction. In Fig. 4 the charge is located in the plane of the paper at the dot, the topological surfaces of the tip and base are represented by the two inner grids, and the corresponding surface-charge distributions are represented by the topmost (σ_1) and lowest (σ_2) grid surfaces, respectively. (All surfaces are symmetric in the plane of the paper.) Figure 5 provides more detail of the surface-charge distribution on the tip. In both figures it is worthwhile to note that the maximum (minimum) values of σ_1 (σ_2) occur at the point in

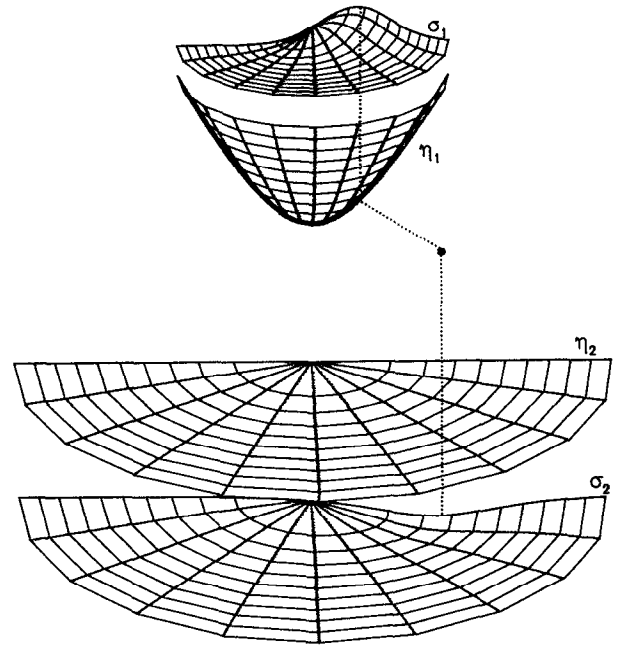


FIG. 4. The surface-charge distributions (σ_1, σ_2) on the tip, base surfaces (η_1, η_2). The charge is located at $\mathbf{x}_c = (\xi_c, \eta_c, \phi_c) = (1.3, 0.5, 0.0)$, and the cone angle (for $\eta_1 = 0.9$) is about 25.8° .

the surface closest to the charge. The maximum value on the tip is $\sigma_1 = 3.523(q/a^2)$, and the minimum value on the base is $\sigma_2 = -2.215(q/a^2)$, where the electron charge $q = -1.6 \times 10^{-19}$ C, and the length-scale a is determined from Eq. (6). For example, if the tip radius of curvature is $20 \text{ \AA}$ and the tip cone angle is $\eta_1 = 0.9$, then $a \sim 94.7 \text{ \AA}$, and the separation distance of the tip and anode is $d_{\text{sep}} \sim 85.3 \text{ \AA}$.

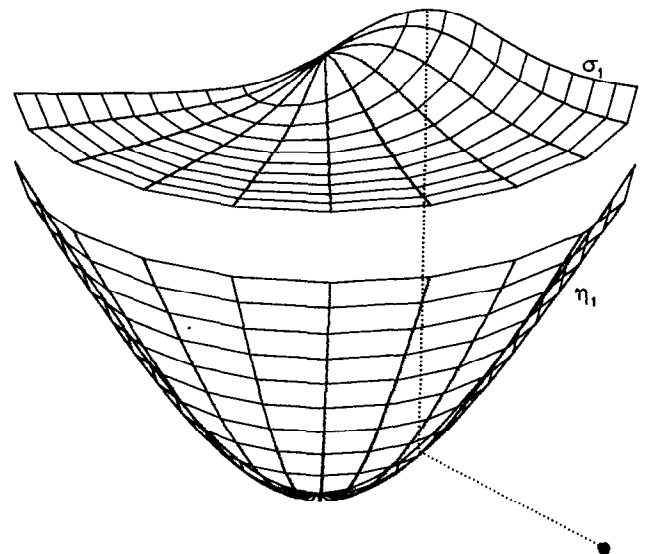


FIG. 5. The surface-charge distribution (σ_1) on the tip (detail of Fig. 4).

VI. SUMMARY

Exact fully three-dimensional solutions for the electrostatic quantities V , Φ , and σ_1, σ_2 for an electron in a tip/base junction are given in this paper in the prolate-spheroidal coordinate system. Very accurate numerical methods for calculating these quantities are described in detail. This result is being used to investigate quantum-size effects in nanoscale electronic devices.

APPENDIX A: CALCULATING THE GAMMA FUNCTION $\Gamma(\mu)$

A strategy described in Arfken (Ref. 8, p. 556) was adapted to create a very accurate scheme for calculating the gamma function $\Gamma(\mu)$ for complex argument μ . Calculating the gamma function from its series definition can produce large round-off errors; however, if the argument μ is very large a very accurate result can be obtained by using Stirling's asymptotic approximation.

In this study a variation (Ref. 11, p. 257, Eq. 6.1.40) of Stirling's asymptotic series,

$$\ln[\Gamma(z)] = \frac{\ln(2\pi)}{2} + \left(z - \frac{1}{2}\right) \ln(z) - z + \frac{B_2}{2z} + \cdots \frac{B_{2n}}{(2n)(2n-1)(z^{2n-1})} + \cdots, \quad (A1)$$

was used to calculate the gamma function for large z . In Eq. (A1) the coefficients B_{2n} are Bernoulli numbers, tabulated in Ref. 11 (p. 810, Table 23.2), and the sum was carried out to the z^{-23} term, inclusive.

In this study, if $|\mu| > 20$, then the gamma function was computed directly from Eq. (A1) by

$$\Gamma(\mu) = \exp[\ln[\Gamma(\mu)]] \quad (A2)$$

On the other hand, if $|\mu| \leq 20$, an intermediate variable $\hat{z}$ was created by

$$\hat{z} = \mu - \text{int}(\mu) + 20, \quad (A3)$$

where the function $\text{int}(\mu)$ returns the largest integer that is less than or equal to μ , generating a variable $\hat{z} > 20$. The gamma function of $\hat{z}$ was obtained from

$$\Gamma(\hat{z}) = \exp[\ln[\Gamma(\hat{z})]], \quad (A4)$$

and then $\Gamma(\mu)$ was obtained from $\Gamma(\hat{z})$ by recursive division, viz.:

$$\Gamma(\mu) = \frac{\Gamma(\hat{z})}{(\mu)(\mu+1)(\mu+2)\cdots(\hat{z}-1)}. \quad (A5)$$

This calculation was carried out in FORTRAN using the COMPLEX*16 variable data types.

APPENDIX B: CALCULATING THE ASSOCIATED CONICAL FUNCTIONS $K_\tau^m(\mu)$

This appendix describes how to calculate associated conical function $K_\tau^m(\mu)$, which are defined by

$$K_\tau^m(\mu) \equiv P_{-\frac{1}{2}+i\tau}^m(\mu); \quad (B1)$$

thus the associated conical function $K_\tau^m(\mu)$ is a special case of the generalized Legendre function $P_n^m(\mu)$ with a complex degree $n \equiv (-\frac{1}{2} + i\tau)$. In generalized Legendre functions the order m must be real, and the degree n and the argument μ may be complex; but for the problem considered in this study the order m is always integer and the argument μ always real, with $-\infty < \mu < \infty$.

A comprehensive text on Legendre functions is Hobson,⁹ which gives numerous series representations for $P_n^m(\mu)$, and the appropriate choice depends principally on the value of the argument μ . For example, in the range $-1 < \mu \leq 1$ the associated conical function has an exponential character with

$$\begin{aligned} P_{-\frac{1}{2}+i\tau}^m(\mu) &\rightarrow 1 & \text{as } \mu \rightarrow 1, & \quad m \equiv 0; \\ P_{-\frac{1}{2}+i\tau}^m(\mu) &\rightarrow 0 & \text{as } \mu \rightarrow 1, & \quad m \neq 0; \\ P_{-\frac{1}{2}+i\tau}^m(\mu) &\rightarrow \infty & \text{as } \mu \rightarrow -1, & \quad \text{all } m. \end{aligned} \quad (B2)$$

On the other hand, for values of $|\mu| > 1$ the associated conical functions have an oscillatory behavior. Because the fundamental character of the solution changes dramatically for $|\mu| \rightarrow 1^+$ this region of the function argument is the most difficult to evaluate with a high degree of numerical precision. After a fair degree of investigation and experimentation with various expressions, the following approach seemed to provide the greatest accuracy.

First, the associated conical functions for order $m > 1$ were determined recursively using the following two expressions from Hobson (Ref. 9, p. 290, Eq. 166):

$$\begin{aligned} P_n^{m+2}(\mu) &= (n-m)(n+m+1)P_n^m - 2(m+1) \\ &\times \frac{\mu}{\sqrt{\mu^2-1}} P_n^{m+1}(\mu) \quad \text{for } |\mu| > 1. \\ P_n^{m+2}(\mu) &= -(n-m)(n+m+1)P_n^m - 2(m+1) \\ &\times \frac{\mu}{\sqrt{1-\mu^2}} P_n^{m+1}(\mu) \quad \text{for } |\mu| \leq 1. \end{aligned} \quad (B3)$$

Because the conical functions are specifically of interest here, $n \equiv (-\frac{1}{2} + i\tau)$ and the recursion relations are

$$\begin{aligned} K_\tau^{m+2}(\mu) &= -[\tau^2 + (m+\frac{1}{2})^2]K_\tau^m(\mu) - 2(m+1) \\ &\times \frac{\mu}{\sqrt{\mu^2-1}} K_\tau^{m+1}(\mu) \quad \text{for } |\mu| > 1, \\ K_\tau^{m+2}(\mu) &= +[\tau^2 + (m+\frac{1}{2})^2]K_\tau^m(\mu) - 2(m+1) \\ &\times \frac{\mu}{\sqrt{1-\mu^2}} K_\tau^{m+1}(\mu) \quad \text{for } |\mu| \leq 1. \end{aligned} \quad (B4)$$

Thus, it is very straightforward to obtain $K_\tau^m(\mu)$ for $m > 1$ once $K_\tau^0(\mu)$ and $K_\tau^1(\mu)$ are evaluated.

To calculate $K_\tau^0(\mu)$ and $K_\tau^1(\mu)$ the following strategy was utilized. If $|\mu| > 1.1$ the following equation (Ref. 9, p. 234, Eq. 68):

$$P_n^m(\mu) = 2^m \frac{\sin((n+m)\pi)}{\cos(n\pi)} \frac{\Gamma(n+m+1)}{\Gamma(n+\frac{3}{2})\Gamma(\frac{1}{2})} z^{-(n+m+1)} \\ \times (\mu^2 - 1)^{m/2} \cdot F(m + \frac{1}{2}, m+n+1, n+\frac{3}{2}, 1/z^2) \\ + 2^m \frac{\Gamma(n+\frac{1}{2})}{\Gamma(n+1-m)\Gamma(\frac{1}{2})} z^{(n-m)} (\mu^2 - 1)^{m/2} \\ \cdot F(m + \frac{1}{2}, m-n, \frac{1}{2}-n, 1/z^2) \quad (B5)$$

was used. In Eq. (B5) $z \equiv \mu + \sqrt{\mu^2 - 1}$, $F(\cdot)$ is the hypergeometric function of the first kind, and since the conical functions are specifically of interest, $n \equiv (-\frac{1}{2} + i\tau)$.

If the argument satisfied the condition that $1.0 < |\mu| < 1.1$ the associated conical function was evaluated as follows. Start with the relation (Ref. 9, p. 235, Eq. 73)

$$P_n^j(\mu) = \frac{2^j}{\Gamma(1-j)} (\mu^2 - 1)^{-j/2} z^{n+j} \\ \cdot F\left(\frac{1}{2}-j, -n-j, 1-2j, 1-\frac{1}{z^2}\right), \quad (B6)$$

and note that, for integer m and $|\mu| > 1$, P_n^m, P_n^{-m} are related by (Ref. 9, p. 205)

$$P_n^m(\mu) = \frac{\Gamma(n+m+1)}{\Gamma(n-m+1)} P_n^{-m}(\mu). \quad (B7)$$

If in Eq. (B6) the order $j \rightarrow -m$ and the resulting expression is incorporated into Eq. (B7), we get

$$P_n^m(\mu) = \frac{\Gamma(n+m+1)}{\Gamma(n-m+1)} \frac{2^{-m}}{\Gamma(m+1)} (\mu^2 - 1)^{jm/2} z^{n-m} \\ \cdot F\left(\frac{1}{2}+m, -n+m, 1+2m, 1-\frac{1}{z^2}\right). \quad (B8)$$

To calculate the conical function from Eq. (B8), again the degree $n \equiv (-\frac{1}{2} + i\tau)$.

Finally, if the argument μ satisfies the condition $|\mu| < 1$ the following expression (Ref. 9, p. 227, Eq. 55)

$$P_n^j(\mu) = \frac{1}{\Gamma(1-j)} \left(\frac{1+\mu}{1-\mu}\right)^{j/2}$$

$$\cdot F[-n, n+1, 1-j, (1-\mu)/2] \quad (B9)$$

was utilized. On the crosscut of the Legendre function (μ real, and $|\mu| < 1$) P_n^m, P_n^{-m} are related by (Ref. 9, p. 230, Eq. 61)

$$P_n^m(\mu) = (-1)^m \frac{\Gamma(n+m+1)}{\Gamma(n-m+1)} P_n^{-m}(\mu). \quad (B10)$$

So, letting $j \rightarrow -m$ in Eq. (40), and substitution of the result into Eq. (B10) gives

$$P_n^m(\mu) = \frac{(-1)^m}{\Gamma(1+m)} \frac{\Gamma(n+m+1)}{\Gamma(n-m+1)} \left(\frac{1+\mu}{1-\mu}\right)^{-m/2} \\ \cdot F[-n, n+1, 1+m, (1-\mu)/2]. \quad (B11)$$

Once again, setting $n \equiv (-\frac{1}{2} + i\tau)$ results in the associated conical function $K_\tau^m(\mu)$.

In this study these conical functions K_τ^m , the gamma functions Γ , and the hypergeometric functions F , were all calculated using the COMPLEX*16 data type in FORTRAN, with the gamma function calculated recursively as described in Appendix A, and the hypergeometric function evaluated using a nested, synthetic-division algorithm.

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