Universal quadratic expansion of the electrostatic tunnelling potential for nanometrically sharp field emitters

Andreas Kyritsakis*

Institute of Technology, University of Tartu, Nooruse 1, 50411 Tartu, Estonia
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Field electron emission from nm-scale objects deviates from the predictions of the classical Murphy-Good theory as the electrostatic potential curves within the tunnelling region. This impels the inclusion of a quadratic term in the potential. At the apex of a tip-like rotationally symmetric surface, this quadratic term is proportional to the (single) local emitter curvature. The present paper generalizes this relation, showing that for any emitter geometry, the coefficient of the quadratic term is given by the mean curvature, i.e. the average of the two principal curvatures.

The most fundamental step in deriving theories of field electron emission is writing an expression for the tunnelling potential. The first theory of field emission by Fowler and Nordheim [1] was based on the exact triangular barrier, while later theories [2, 3] included the image potential corrections to the barrier. In all these cases, the electrostatic potential has been approximated to be linear with the distance from the surface z, i.e. \( \Phi(z) = Fz \), with \( F \) being the local electric field at the emission point.

However, it is well-known that this approximation is not valid for emitters with nanometric radii of curvature, as has been shown both theoretically and experimentally [4–8]. In such cases the potential becomes curved within the tunnelling region and the linear expansion is insufficient as higher order terms become significant. Kyritsakis and Xanthakis [5] used a quadratic expansion of the electrostatic potential

\[
\Phi(z) = Fz + \frac{Fz^2}{R} + O(z^3), \quad z \to 0
\]

and derived a generalized Fowler-Nordheim-type equation for the emission current density \( J \) as a function of the local field \( F \), the work function \( \phi \), and the quadratic term parameter \( R \):

\[
J(F, \phi, R) = a \frac{F^2}{\phi} \left[ \frac{1}{\lambda_d(f)} + \frac{\phi}{\epsilon FR} \psi(f) \right]^{-2} \exp \left[ b \frac{\phi^{3/2}}{F} \left( \nu(f) + \omega(f) \frac{\phi}{\epsilon FR} \right) \right].
\]

In the above equation, \( f \equiv (e^3/4\pi\epsilon_0)(F/\phi^2) = (1.439964 \text{ eV}^{-1} \text{ nm}^{-1}) (F/\phi^2) \) is the reduced field strength, \( \nu(f), \omega(f), \lambda_d(f), \psi(f) \) are known and tabulated functions [5], and \( a \equiv e^3/(16\pi^2\hbar) \approx 1.544433 \times 10^{-6} \text{ eV} \text{ V}^{-2/3} \), \( b \equiv 4\sqrt{2\pi}/3e\hbar \approx 6.830890 \text{ (eV)}^{-3/2} \text{ eV nm}^{-1} \) are universal constants, also known as the first and second Fowler-Nordheim constants respectively.

The resulting current density vs field plot deviates significantly from the typical straight-line Fowler-Nordheim behavior, with a curvature that scales with the quadratic parameter \( 1/R \). It was also shown that at the apex of a typical rotationally symmetric emitting nanotip, which is an umbilic point [9] of the emitting surface, the quadratic parameter \( R \) is equal to the (single) local radius of curvature. Since in such tips most of the emission is coming from the vicinity of the apex, approximating the quadratic term as the apex curvature yields a reasonably good approximation for the emission current.

However, non-tip-like emitters that are not rotationally symmetric and cannot be described by the above approximation have started being studied a lot. Especially edge-type emitters from two-dimensional materials such as nanosheets and nanoflakes have recently attracted significant interest [10–16]. Furthermore, modern numerical models of field emission [17–20] need to resolve the emission distribution at each point of the emitter separately. In Refs. [18, 19], this was tackled by calculating numerically the whole electrostatic potential function along the emission path. However, this is computationally expensive as it requires very high numerical accuracy in the tunnelling region. Deriving a general expression for the quadratic emission term can be used both for the accurate theoretical calculation and the precise and computationally efficient simulation of the emitted current density from emission surfaces with arbitrary geometry.

Biswa et. al. [21] calculated the quadratic term for a few specific geometries that have known analytical solutions. They found that the quadratic parameter \( R \) is equal to the second (smaller) principal radius of curvature \( R_2 \), i.e. \( R = R_2 \). This paper gives a general and rigorous derivation of the electrostatic electrical expansion for any point at any continuous emitter surface, showing that the correct expansion term involves the radius of mean curvature [22], i.e. \( R = R_m \). This result necessarily renders the results by Biswa et. al. [21] erroneous. A brief revision of their derivation pinpoints a subtle mathematical error that yielded the result \( R = R_2 \).

In order to prove the above statement \( R = R_m \), let me start by considering an equipotential emitting surface and an arbitrary point \( O \) on it, as shown in figure 1. Without loss of generality, I define a cartesian coordinate system centered at \( O \), with its \( \hat{z} \) direction being perpendicular to the surface, i.e. \( \hat{z} \equiv \hat{n} \). This coordinate
system is known in differential geometry as the Darboux frame of an arbitrary curve belonging to the surface. In the vicinity of $O$, the surface can be described by the Monge patch [23] \( r(u, v) = (u, v, g(u, v)) \). The perpendicular vector at a given point of the surface is given by

\[
\hat{n} = \frac{r_u \times r_v}{|r_u \times r_v|} = \frac{(-g_u, -g_v, 1)}{\sqrt{g_u^2 + g_v^2 + 1}}, \tag{3}
\]

where subscripts denote partial derivatives. Given the selection of the coordinate system, \( \hat{n} \equiv \hat{z} \), it is \( g_u = g_v = 0 \) at \( O \). In the Monge patch representation of the surface, the mean curvature is given by [23]

\[
H \equiv \frac{(1 + g_u^2)g_{uu} + 2g_u g_v g_{uv} + (1 + g_v^2)g_{vv}}{2(1 + g_u + g_v)^{3/2}}. \tag{4}
\]

In the chosen coordinate system, the above expression evaluated at \( O \), where \( g_u = g_v = 0 \), simplifies into

\[
H(O) \equiv \frac{1}{R_m} = \frac{g_{uu} + g_{vv}}{2}. \tag{5}
\]

Consider now the potential along the \( z \) axis \( \Phi(x = 0, y = 0, z) \), assuming that the surface \( (u, v, g(u, v)) \) is equipotential and (without loss of generality) grounded, i.e.

\[
\Phi(u, v, g(u, v)) = 0. \tag{6}
\]

Expanding \( \Phi(z) \equiv \Phi(0, 0, z) \) in a Taylor series around \( O \), it yields

\[
\Phi(z) = Fz + \frac{1}{2}\Phi_{zz}(O)z^2 + O(z^3), z \to 0 \tag{7}
\]

where I have simplified by substituting \( \Phi(O) = 0 \), and \( \Phi_z(O) \equiv F \). From this expansion, it yields that the quadratic parameter \( R \) of eq. (1) is given by

\[
R = \frac{2F}{\Phi_{zz}(O)}. \tag{8}
\]

Let us now take the derivatives of eq. (6) with respect to \( u \). It yields

\[
\Phi_x + \Phi_z g_u = 0. \tag{9}
\]

Writing the same equation for the \( v \)-derivatives and evaluating at \( O \) where \( g_u = g_v = 0 \), it yields

\[
\Phi_x(O) = \Phi_y(O) = 0. \tag{10}
\]

In order to write the second \( u \)-derivatives of equation (6), eq. (9) needs to be differentiated. It yields

\[
\Phi_{xx} + 2g_u \Phi_{xz} + \Phi_{zz}g_u^2 + \Phi_{z}g_{uu} = 0. \tag{11}
\]

Evaluating eq. (11) at \( O \), and performing the same calculations for the \( v \)-derivatives yields

\[
\Phi_{xx}(O) = -Fg_{uu}(O), \quad \Phi_{yy}(O) = -Fg_{vv}(O). \tag{12}
\]

Now considering that the electron emission is occurring in vacuum (disregarding any space charge effects), the electrostatic potential \( \Phi \) satisfies the Laplace equation, i.e.

\[
\Phi_{zz} = -\Phi_{xx} - \Phi_{yy}. \tag{13}
\]

Substituting \( \Phi_{x}x, \Phi_{y}y \) from (12) yields

\[
\Phi_{zz}(O) = F(g_{uu} + g_{vv}), \tag{14}
\]

which in view of (8) gives the central result of this paper:

\[
R = \frac{2}{g_{uu}(O) + g_{vv}(O)} = \frac{1}{H(O)} = R_m \tag{15}
\]

Note that the above equation is general. The selection of the point \( O \) is absolutely arbitrary and the only assumption about the shape of the equipotential surface is that it is mathematically smooth (differentiable).

A comment is worthy on the result obtained for ellipsoid and hyperboloid emitters by Biswas et. al. [21], which is contradicting the above general expression. Revisiting the derivation of reference [21], it is evident that substituting their eq. [21] into the expression of the potential as a function of the spheroidal coordinates does not yield their eq. (10). The truncated \( O(\Delta s^2) \) terms of their eq. (8) should yield an \( O(\Delta s^2) \) contribution, which has been completely disregarded. Considering this contribution properly, would lead to the general result of eq. (15).

To confirm the latter and validate the main result of this paper, I shall calculate \( R \) for the specific hyperboloid tip geometry, which is addressed in chapter IIB...
of Ref. [21]. The electrostatic field is given as a function of the prolate spheroidal coordinates \( \eta, \xi \) (defined as in Ref. [21]) is

\[
\Phi(\eta, \xi) = V \left( 1 - \log \frac{1 - \xi^2}{1 + \xi^2} \right),
\]

where \( \xi = \xi_0 < 0 \) defines the equipotential surface \( \Phi = 0 \) of the emitter and \( \xi = 1 \) defines the anode where \( \Phi = V \). The corresponding electric field perpendicular to the emitter surface is

\[
F(\eta, \xi_0) = \frac{2V}{c \sqrt{(1 - \xi_0^2) \left( \eta^2 - \xi_0^2 \right)}} \left( \frac{c}{\xi_0} \right),
\]

where \( c \) is the focal length of the hyperboloid.

As in the general case, I define the \( z \)-coordinate at an arbitrary point \((\eta, \xi_0)\) on the emitter surface as the distance from the point along the perpendicular line. Using the general definition of eq. (8), it yields

\[
R = \frac{1}{2F} \frac{\partial F}{\partial \xi},
\]

where \( h_\xi = c\sqrt{\eta^2 - \xi_0^2} \) is the metric factor. Evaluating eq. (18) by differentiating (17) yields

\[
R = -2c \left( \frac{\eta^2 - \xi_0^2}{\xi_0} \right)^{3/2} \sqrt{1 - \xi_0^2},
\]

The principal radii of curvature of the emitter hyperboloid are [21]

\[
R_1 = -\frac{c}{\xi_0} \left( \frac{\eta^2 - \xi_0^2}{\xi_0} \right)^{3/2} \sqrt{1 - \xi_0^2},
\]

\[
R_2 = -\frac{c}{\xi_0} \sqrt{(\eta^2 - \xi_0^2)(1 - \xi_0^2)}.
\]

After a few algebraic manipulations, it yields

\[
R_m = \frac{1}{2R_1} + \frac{1}{2R_2} = -\frac{2c \left( \frac{\eta^2 - \xi_0^2}{\xi_0} \right)^{3/2} \sqrt{1 - \xi_0^2}}{\xi_0 \left( 2\xi_0^2 + \eta^2 \right)}
\]

which confirms the main result of this paper, i.e. \( R = R_m \). Note that the minus sign in the above expressions come from the fact that \( \xi_0 < 0 \).

In conclusion, this paper gives a rigorous proof that the quadratic term of the expansion of the electrostatic potential along a path perpendicular to an arbitrary equipotential surface, is proportional to the local mean curvature of the surface, i.e. the average of its two principal curvatures. This general result can be used to calculate accurately field electron emission from surfaces of any geometry without having to extract the entire potential distribution in the tunnelling region. Finally, it corrects the wide-spread misconception in the literature [21] that connects the quadratic term to the second principal curvature of the surface.

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* akyritos1@gmail.com; andreas.kyritsakis@ut.ee

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