Exact mathematical solution for the principal field emission correction function v used in Standard Fowler-Nordheim theory

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The Standard Fowler-Nordheim (FN) type Equation, as derived from Murphy and Good's analysis [1] of tunnelling through a Schottky-Nordheim (SN) barrier [2], is normally written:

$$J = t_F^{-2} a \phi^{-1} F^2 \exp\{-v_F b \phi^{3/2}/F\} , \tag{1}$$

where the symbols have their usual meanings. The subscript "F" labels values that apply to a tunnelling barrier of unreduced height ϕ, and v_F and t_F are particular values of mathematical functions called v and t. t and other mathematical functions used in Standard FN-type theory may be derived from v and its derivatives, so primary mathematical interest is in this "Principal Field Emission Correction Function" v.

It has become clear that the best long-term strategy is to create a formal separation between the physical and mathematical aspects of eq. (1), because: (a) some (though not all) of the formulae associated with the applications of eq. (1) are special versions of more general physical formulae applicable to any well-behaved tunnelling barrier; and (b) the mathematics of v is applicable to various different tunnelling-barrier problems.

On the mathematical side, we introduce a mathematical variable l', defined in terms of the "elliptic parameter" m [3] used in elliptic-function theory by

$$l' = [(1-m)/(1+m)]^2 , \tag{2}$$

and derive an exact series expansion for $v(l')$. l' is related to the Nordheim parameter by $l'=y^2$.

On the physical side, we replace eq. (1) by the General-Barrier FN-type Equation [4]

$$J = \tau_F^{-2} a \phi^{-1} F^2 \exp[-\nu_F b \phi^{3/2}/F] , \tag{3}$$

where the physical parameter ν is the tunnelling-exponent correction factor, and τ is the physical parameter defined in Ref. [4]. Eq. (3) is applicable to any well-behaved barrier, including the real tunnelling barrier (assuming this is well-behaved). We consider ν_F and τ_F to be functions of the real, physical, scaled barrier field $f = F/F_\phi$ where F_ϕ is the real barrier field necessary to reduce the real tunnelling barrier from height ϕ (at F=0) to zero (at F=F_ϕ).

When, in Standard Theory, the barrier is modelled as a Schottky-Nordheim barrier, then F_ϕ is estimated using Schottky's (1923) formula $F_\phi^{SN}=(e^3/4\pi\varepsilon_0\phi^2)$, and f is estimated as $f^{SN}=F/F_\phi^{SN}$. In these circumstances the mathematics shows that $l'=f^{SN}$. So, for this barrier model, the real (unknown) numerical value of $\nu_F(f)$ is modelled/estimated by $v(f^{SN})$.

An expression for v in terms of the complete elliptic integrals K and E is known [1,5]. From this it can be found [6] that $v(l')$ is a particular solution of the ordinary differential equation (ODE)

$$l'(1-l')\mathrm{d}^2W/\mathrm{d}l'^2 = nW, \tag{4}$$

when the index $n = {}^3/_{16}$. This ODE appears to be new in elliptic-function theory and in mathematical physics, and we provisionally call it the "Super-elliptic Equation of index n". By using the method of Frobenius (e.g., [7]), we have shown that two independent solutions, $W_A(l')$ and $W_C(l')$, of this Super-elliptic Equation may be expressed as the series expansions

$$W_{\mathrm{A}}(l') = l' \sum_{i=0}^{\infty} a_i l'^i, \qquad W_{\mathrm{C}}(l') = l' \ln l' \sum_{i=0}^{\infty} a_i l'^i + \sum_{i=0}^{\infty} b_i l'^i, \tag{5}$$

where $a_0 = 1$, $b_0 = 1/n$, $b_1 = -1$, and the other coefficients are given by the recurrence relations

$$a_{i+1} = \frac{i(i+1)+n}{(i+1)(i+2)} a_i\ , \ i \geq 0; \qquad b_{i+1} = \frac{(2i-1)a_{i-1} - (2i+1)a_i + \{(i-1)i+n\}b_i}{i(i+1)},\ i \geq 1. \tag{6}$$

The general solution can be written $W = AW_{\mathrm{A}} + CW_{\mathrm{C}}$, where A and C are arbitrary constants.

The boundary conditions on $v(l')$ are that $v(0)=1$, and that [6]

$$\lim(l'\to 0)\ \mathrm{d}v/\mathrm{d}l' \ = \ -{}^{9}/_{8}\ln 2 \ + \ {}^{3}/_{16} \lim(l'\to 0)\ \ln l'\ . \tag{7}$$

With $n={}^{3}/_{16}$, these lead to the results: $A = -{}^{9}/_{8}\ln 2$, $C = {}^{3}/_{16}$, and

$$v(l') \ = \ 1 + \sum_{i=0}^{\infty} (Aa_i + Cb_{i+1} + Ca_i \ln l') l'^{i+1}. \tag{8}$$

The first few terms of this expansion, first found by the software package MAPLE™ [8], are:

$$v(l') = 1 - \left(\tfrac{9}{8}\ln 2 + \tfrac{3}{16}\right)l' - \left(\tfrac{27}{256}\ln 2 - \tfrac{51}{1024}\right)l'^2 - \left(\tfrac{315}{8192}\ln 2 - \tfrac{177}{8192}\right)l'^3 - \ldots + \left(\tfrac{3}{16} + \tfrac{9}{512}l' + \tfrac{105}{16384}l'^2 + \ldots\right)l' \ln l' \tag{9}$$

With coefficients evaluated to 5 decimal places, this can alternatively be put into form (10), which is explicitly exact at $l'=0$ and $l'=1$ and has good convergence properties:

$$v(l') = (1-l')\,(1+0.03271l' + 0.00941l'^2 + \ldots) + l'\ln l'\,(0.18750+0.01758l'+0.00641l'^2+ \ldots). \tag{10}$$

This in turn suggests looking for numerical approximation formulae of the form

$$v_j(l') \approx (1-l')\left\{1+\sum_{i=1}^{j} p_i l'^i\right\} + l'\ln l' \sum_{i=1}^{j} q_i l'^{i-1}. \tag{11}$$

i	p_i	q_i
1	0.032 705 304 46	0.187 499 344 1
2	0.009 157 798 739	0.017 506 369 47
3	0.002 644 272 807	0.005 527 069 444
4	0.000 089 871 738 11	0.001 023 904 180

Taking j=4, and minimising squared error, yields the coefficients in the adjacent table, and a formula with absolute error $|\varepsilon| \leq 8\times10^{-10}$. This performance exceeds, by a factor of about 400, that of the best existing numerics of equivalent complexity.

Clearly, the approximation formula $v(l') \approx 1-l'+{}^{1}/_{6}l'\ln l'$ reported earlier [8], which has $|\varepsilon| \leq 3.5\times10^{-3}$, is a particularly simple case of form (11). It is not quite the optimum formula of its type; its merit is its algebraic simplicity, coupled with accuracy fit for purpose.

Important results here are that $v(l')$ obeys eq. (4), and its solution by the method of Frobenius. The outcome provides sound mathematical grounds for holding that l' (rather than the Nordheim parameter y) is the natural mathematical variable to use, and hence that "scaled barrier field" is the natural physical variable. The Frobenius method shows that fractional powers of l' are not needed and that terms in $\ln l'$ are intrinsic to the correct mathematical solution, and to good formulae for v. This is the main reason for the superior performances.

In summary, this work puts the mathematics of the Schottky-Nordheim barrier onto a more complete and fully respectable basis. It also opens the way to new developments.

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