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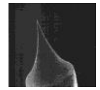
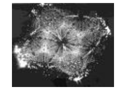


High-Electric-Field Nanoscience



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WHY USING THE NORDHEIM PARAMETER *y* IN THE MATHEMATICS OF THE SPECIAL MATHEMATICAL FUNCTION "v" USED IN FIELD EMISSION THEORY SHOULD NOW BE REGARDED AS MATHEMATICALLY PERVERSE

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Introduction

Murphy-Good (MG) field electron emission (FE) theory is based on tunneling through a planar image-rounded barrier, often known as a Schottky-Nordheim (SN) barrier. In MG FE theory one can write the following expression for the emission current I_e in terms of the local work function ϕ and a characteristic local surface field F_C near the emitter apex:

$$I_e = Aa\phi^{-1}F_C^{2}\exp[-b\mathrm{v}_F\phi^{3/2}/F_C] \ .$$

Here, a and b are the Fowler-Nordheim constants, A is an area-like quantity, and v_F is an appropriate particular value (appropriate to a barrier defined by ϕ and F_C) of a special mathematical function (SMF) usually just called "v".

It has been know since 2008 that the SMF "v" is a very special solution of the Gauss Hypergeometric Differential Equation (HDE); consequently I now consider it best mathematical practice to take "v" as a function of the independent variable in the the Gauss HDE, which I denote by x and call the Gauss variable. Thus I now write $\mathrm{v}(x)$.

This replaces the "legacy convention" of expressing "v" as a function of the Nordheim parameter y [$=+\sqrt{x}$].

Introduction

In recent years I have been arguing that we should make a separation between the mathematics of the SMF "v" and its use in modelling FE and other physical phenomena.

I have also been arguing that continued use of the Nordheim parameter y in the *mathematics* of the SMP "v" should now be considered as mathematically perverse.

When applying the SMF $v(x)$ to modelling FE, using MG FE theory, there are (as just indicated) two possible conventions.

(a) The "21st century convention" of setting x equal to the scaled field f defined by

$$f \;=\; (e^3/4\pi\varepsilon_0)\,\phi^{-2}\,F\,.$$

(b) The "legacy convention" of setting x equal to the Nordheim parameter y_F defined by $y_F=+\sqrt{f}\,.$

Both conventions are legitimate in modelling, but my view is that the "21st century convention" is more useful for experimentalists.

Using sin(x) *to demonstrate perversity*

Now suppose that there is a group of people who think it would be better if the series expansion contained only even terms (lets call them "even-power (ep) people").

This can be achieved by setting $x=y^2$ in the series expansion, thereby defining a new SMF epsin(y) by

$$\mathrm{epsin}(y) = y^2 - y^6/3! + y^{10}/5! - \ldots$$

The rule for calculating the sines of angles now becomes: "take the angle θ, find its square root $\theta^{1/2}$, and substitute $y=\theta^{1/2}$ into the SMF epsin(y)" .

This procedure will work, but probably most people would regard as mathematically perverse, as compared with the normal procedure.

Also, if you reformulate the defining equation in terms of y, rather than x, it becomes significantly more complicated, as

$$y^2\, d^2W/dy^2 - dW/dy + 4y^3 W = 0\ .$$

Mathematical perversity relating to v

As a result of mathematical developments in the theory of "v" that took place in the period 2006 to 2010, we now know: (a) that "v" is a particular solution of the defining equation

$$x(1-x)\mathrm{d}^2W/\mathrm{d}x^2 = (3/16)W \;;$$

(b) that this defining equation is a special case of the Gauss Hypergeometric Equation, so "x" is the Gauss variable; (c) that an exact analytical expression for v(x) exists and is known; and (d) that an exact series expansion for v(x) exists and is known.

v(x) is the particular solution of above defining equation that meets the (unusual) boundary conditions:

$$\mathrm{v}(0) = 1; \quad \lim(x\to 0)\{\mathrm{dv}/\mathrm{d}x - (3/16)\ln x\} = -(9/8)\ln 2 \,.$$

Mathematical perversity relating to v

As before, if the variable x is set equal to y^2, then the defining equation gets significantly more complicated:

$$y\,(1-y^2)\,\mathrm{d}^2W/\mathrm{d}y^2 \;-\; (1-y^2)\,\mathrm{d}W/\mathrm{d}y \;-\; (3/4)\,yW \;=\; 0\,.$$

This equation is not obviously related to the Gauss HDE, and would be difficult to solve. Hence, use of y rather x is, as in the sin(x) case, mathematically perverse.

There is another indicator of the unsuitability of y in the mathematics. One of the exact series expansions for v(x) has the form

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

Note that no terms in $x^{1/2}$ appear in this exact series expansion. This shows that x (rather than y [= $x^{1/2}$]) is the natural mathematical variable to use for the argument of v.

The merits of using f (not y_F) in modelling

Advantages of using scaled fields are:

- ✓ **can be measured with a FN plot, more accurately than fields;**
- ✓ **useful for discussing emitter current-voltage behaviour;**
- ✓ **unifying approach for the different conventions for describing fields;**
- ✓ **for ideal emitters, are also scaled voltages and macroscopic fields;**
- ✓ ***f*-ranges are more uniform as between materials than field-*F* ranges;**
- ✓ **proportional to barrier field, so easy to convert back;**
- ✓ **can be used to characterize onset of effects, e.g. turn-on or melting;**
- ✓ **hence are used in the orthodoxy test.**

The merits of using f (not y_F) in modelling

Criteria of emitter behaviour were noted long ago by Dyke and Dolan for one of their experimental systems. These criteria can be expressed in terms of characteristic ("emitter-apex") values (f_C) of scaled field, as shown in the table below.

[These f_C -values apply to room-temperature emission, in traditional single-pointed-emitter experimental geometry, for a tungsten emitter (with assumed work function 4.50 eV). For simplicity, the local current density J_{kC}^{SN} is calculated using (0 K) SN-barrier theory.]

Criterion	f_C	J_{kC}^{SN} (A/m²)
Emission onset	0.20	~ 8.7×10^4
Safe steady-current limit	0.34	~ 2.3×10^9
Onset of space-charge effects	0.49	~ 2.3×10^{11}
Safe pulsed-current limit	0.60	~ 1.7×10^{12}
Breakdown of (0 K) MG theory	~ 0.8	~ 1.6×10^{13}
Apex barrier pulled down to Fermi level.	1.00	–

The Burgess, Kroemer & Houston (BKH) table

TABLE I. Values of $v(y)$ and $s(y)$.

y	$v(y)$	$s(y)$
0	1.0000	1.0000
0.05	0.9948	0.9995
0.1	0.9817	0.9981
0.15	0.9622	0.9958
0.2	0.9370	0.9926
0.25	0.9068	0.9885
0.3	0.8718	0.9835
0.35	0.8323	0.9777
0.4	0.7888	0.9711
0.45	0.7413	0.9637
0.5	0.6900	0.9554
0.55	0.6351	0.9464
0.6	0.5768	0.9366
0.65	0.5152	0.9261
0.7	0.4504	0.9149
0.75	0.3825	0.9030
0.8	0.3117	0.8903
0.85	0.2379	0.8770
0.9	0.1613	0.8630
0.95	0.0820	0.8483
1.	0	0.8330

Many approximations for v(*y*) in the literature seem to have been derived by fitting to this table. [Phys. Rev. 90 (1953) 515.]

One of these is the 1962 Charbonnier and Martin approximation, which in terms of *x* is: $v_{CM}(x) = 0.956 - 1.062\,x$.

Modern derivation of the CM approximation

The SMF u(x) is defined in terms of v(x) by

$$u(x) \;=\; -\mathrm{d}v/\mathrm{d}x\;.$$

The SMF s(x) is defined in terms of v(x) by

$$s(x) \;=\; v(x) - x\mathrm{d}v/\mathrm{d}x \;=\; v(x) + x\,u(x)\;.$$

Hence we conclude that

$$v(x) \;=\; s(x) \;-\; x\,u(x),$$

and that when this is applied to Murphy-Good FE theory, then the relation becomes

$$v(f) \;=\; s(f) \;-\; f\,u(f)$$

Both u(f) and s(f) are slowly varying functions of f, so in the vicinity of some particular scaled field value f_0 we can write (approximately)

$$v(f\,) \;\approx\; s(f_0) \;-\; u(f_0)\,f.$$

If we take a typical "mid-range operating value" as f_0=0.25, then a high precision spreadsheet yields u(0.25) = 1.062, s(0.25) = 0.9554, and results in the formula

$$v(f\,) \;=\; 0.9554 - 1.062\,f\;.$$

Obviously, this is very close to the Charbonnier and Martin result.

Thanks for your attention

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